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FILE LAST UPDATED: 21 Apr 2003  (20030421/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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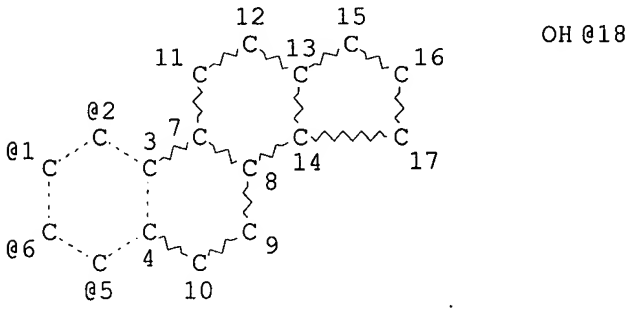


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NUMBER OF NODES IS  18

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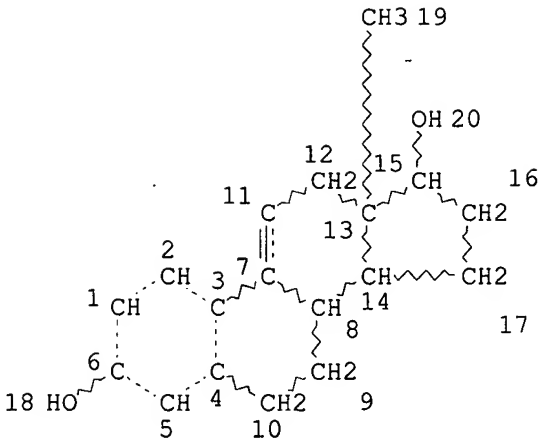

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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L17 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L16

=>
=> d ibib abs hitrn l17 1-37

L17 ANSWER 1 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:717656 HCAPLUS
DOCUMENT NUMBER: 138:50028
TITLE: Development and validation of an average mammalian estrogen receptor-based QSAR model
AUTHOR(S): Mekenyan, O.; Kamenska, V.; Serafimova, R.; Poellinger, L.; Brouwer, A.; Walker, J.
CORPORATE SOURCE: Laboratory of Mathematical Chemistry, University "As. Zlatarov", Bourgas, 8010, Bulg.
SOURCE: SAR and QSAR in Environmental Research (2002), 13(6), 579-595
CODEN: SQERED; ISSN: 1062-936X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Development and evaluation of quant. structure activity relationships (QSARs) for predicting estrogen receptor binding from chem. structure requires reliable algorithms for three-dimensional (3D) QSAR anal. and establishment of structurally diverse training sets of chems. whose modes of action and measures of potency are well defined. One approach to selecting an appropriate training set is to minimize the biol. variability in the model development, by using structurally restricted data sets. A second approach is to extend the structural diversity of chems. at the cost of increased variability of biol. assays. In this study, the second approach was used by organizing a training set of 151 chems. with measured human alpha Estrogen Receptor (ER.alpha.), mouse uterine, rat uterine, and MCF7 cell Relative Binding Affinities (RBAs). The structurally augmented training set was submitted to a 3D pattern recognition anal. to derive a

model for av. mammalian ER binding affinity by employing the COmmon REactivity PAttern (COREPA) approach. Elucidation of this pattern required examn. of the conformational flexibility of the compds. to reveal areas in the multidimensional descriptor space, which are most populated by the conformers of the biol. active mols. and least populated by the inactive ones. The approach is not dependent upon a predetd. and specified toxicophore or an alignment of conformers to a lead compd. Reactivity patterns assocd. with mammalian ER binding affinity were obtained in terms of global nucleophilicity (EHOMO), interat. distances between nucleophilic sites, and local nucleophilicity (charges or delocalizabilities) of those sites. Based on derived patterns, descriptor profiles were established for identifying and ranking compds. with RBA of >150, 150-10, 10-1 and 1-0.1% relative to 17.beta.-estradiol. Specificity of reactivity profiles was found to increase gradually with increasing affinities assocd. with RBAs ranges under study. Using the results of this anal., an exploratory expert system was developed for use in ranking relative mammalian ER binding affinity potential for large chem. data sets. The validity of the RBA predictions were confirmed by independent development and comparison with measured RBA values.

IT 791-69-5
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(development and validation of an av. mammalian estrogen receptor-based QSAR model)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:391545 HCAPLUS
DOCUMENT NUMBER: 136:386298
TITLE: Preparation of enantiomeric estrogen derivatives containing unsaturated bonds in conjugation with the terminal or A ring as potential cytoprotective and neuroprotective agents
INVENTOR(S): Covey, Douglas F.
PATENT ASSIGNEE(S): Washington University, USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040032	A2	20020523	WO 2001-US47262	20011105
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002028891	A5	20020527	AU 2002-28891	20011105
US 2002132802	A1	20020919	US 2001-8567	20011105

PRIORITY APPLN. INFO.: US 2000-249580P P 20001117
WO 2001-US47262 W 20011105

OTHER SOURCE(S): MARPAT 136:386298
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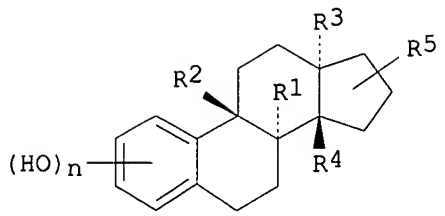

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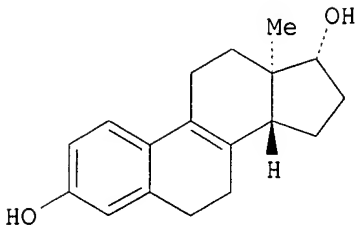


II

AB The title compd. I (1 or more unsatd. bonds in conjugation with the arom. A-ring between C's 6,7,8,9 or 11; n = 1-4; R1, R2 = H, alkyl; R3 = H, substituted or unsubstituted hydrocarbyl, halo, amido, sulfate, nitrate; R4 = H, alkyl; R5 = H, hydroxy, oxo, substituted or unsubstituted hydrocarbyl, heterocycloakyl, heterocycloalkenyl, halo, amido, sulfate, nitrate; carbon 17 and carbon 3 are not hydroxy substituted when n = 1, the compd. does not contain at least one unsatd. bond in conjugation with the arom. A-ring, R1, R2, R4 = H, and R3 = Me) were prepd. as potential cytoprotective and neuroprotective agents. Thus, ent-(17.beta.)-17-(1,1-dimethylethoxy)-3-methoxyestra-1,3,5(10),8-tetraene was treated with TiCl4 followed by redn. with diisobutylaluminum hydride to give ent-(17.beta.)-3-methoxyestra-1,3,5(10),8-tetraen-17-ol (II). In an assay for neuroprotection of HT-22 cells against glutamate induced cell death II had and ED50 of 1.23 .mu.M in the presence of 10 mM glutamate and 1.85 .mu.M at 20 mM glutamate.

IT **300853-09-2P**, ZYC 10 **428506-98-3P**, ZYC 12
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of enantiomeric estrogen derivs. contg. unsatd. bonds in conjugation with the terminal or A ring as potential cytoprotective and neuroprotective agents)

IT **791-69-5**, ZYC 1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of enantiomeric estrogen derivs. contg. unsatd. bonds in conjugation with the terminal or A ring as potential cytoprotective and neuroprotective agents)

L17 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:828235 HCAPLUS
DOCUMENT NUMBER: 136:161484
TITLE: Specific Photoaffinity-Labeling of Tyr-50 on the Heavy Chain and of Tyr-32 on the Light Chain in the Steroid Combining Site of a Mouse Monoclonal Anti-Estradiol Antibody Using C3-, C6-, and C7-Linked 5-Azido-2-nitrobenzoylamidoestradiol Photoreagents
AUTHOR(S): de Ravel, Marc Rolland; Blachere, Thierry; Delolme, Frederic; Dessalces, Guy; Coulon, Stephane; Baty, Daniel; Grenot, Catherine; Mappus, Elisabeth; Cuilleron, Claude Y.
CORPORATE SOURCE: Institut National de la Sante et de la Recherche Medicale, Hopital Debrousse, Lyon, 69322, Fr.
SOURCE: Biochemistry (2001), 40(49), 14907-14920
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A mouse monoclonal anti-7-(O-carboxymethyl)oximinoestradiol antibody 9D3, raised against the same immunogen as that employed for generating the

reported anti-estradiol antibody 15H11, was found to exhibit an opposite specificity profile with a much stronger recognition of the D-ring than of the A-ring extremity of the steroid, but a similar lack of specificity for both 6- and 7-positions of the B-ring. This antibody was photoaffinity-labeled with five (5-azido-2-nitrobenzoyl)amido (ANBA) derivs. of [17.alpha.-3H]estradiol, synthesized from 3-aminoethyloxy, 3-(aminoethylamido)carboxymethyloxy, 6.alpha.- and 6.beta.-amino, and 7-[O-(aminoethylamido)carboxymethyl]oximino precursors. After tryptic digestion, the radioactive peptides on L and H chains were immunopurified with the immobilized antibody 9D3, sepd. by reversed-phase liq. chromatog., sequenced, and characterized by mass spectrometry, including post-source decay-matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. The long 3-(ANBA-ethylamido)carboxymethyl ether photoreagent was found to label TyrL-32 (on CDR L1), whereas no labeling was obsd. with the shorter 3-deriv., a result in agreement with a binding pocket large enough to explain the high cross-reactivity with estradiol 3-conjugates. The two 6.alpha.- and 6.beta.-ANBA-estradiol isomers, as well as the 7-[O-(ANBA-ethylamido)carboxymethyl]oximinoestradiol photoreagent derived from the steroid hapten, labeled the same TyrL-32 residue. The 6.beta.-ANBA epimer also labeled TyrH-50 (at the basis of CDR H2). These expts. indicate that TyrL-32 is freely accessible from the three C3, C6, and C7 positions, all presumed to be exposed to solvent, while TyrH-50 is probably located on the .beta.-face of estradiol. These results, obtained in soln., provide exptl. data useful for mol. modeling of the steroid-antibody complex.

IT **791-69-5**, .DELTA.9,(11)-Estradiol
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(specific photoaffinity-labeling of Tyr-50 on heavy chain and of Tyr-32 on light chain in steroid combining site of mouse monoclonal anti-estradiol antibody using C3-, C6-, and C7-linked 5-azido-2-nitrobenzoylamidoestradiol photoreagents)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:443930 HCAPLUS
DOCUMENT NUMBER: 137:140672
TITLE: Pre-processing of three-way data by pulse-coupled neural networks-an imaging approach
AUTHOR(S): Magnus Aberg, K.; Jacobsson, S. P.
CORPORATE SOURCE: Department of Analytical Chemistry, Stockholm University, Stockholm, SE-106 91, Swed.
SOURCE: Chemometrics and Intelligent Laboratory Systems (2001), 57(1), 25-36
CODEN: CILSEN; ISSN: 0169-7439
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new method for pre-processing three-dimensional data to model quant. structure-retention relationships (QSRR) is presented. The pre-processing of three-dimensional images of mols. is done with a pulse-coupled neural network (PCNN). The PCNN is capable of transforming an image to a short time series representation of the mol., which is more suitable for QSRR modeling with partial least squares than the original data. The method was developed and tested on a steroid data set of 24 compds. with reversed-phase high-performance liq. chromatog. retention data. The QSRR models are stable with respect to the parameters of the PCNN. Test set correlations (q2) of 0.95 and cross-validated r2 of about 0.95 are readily obtained.

IT **791-69-5**, 9,11-Dehydroestradiol
RL: PRP (Properties)
(an imaging approach to pre-processing of three-way data by

pulse-coupled neural networks for QSRR of estranes)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:416751 HCAPLUS
DOCUMENT NUMBER: 135:10053
TITLE: Transdermal drug delivery systems with improved oxidative stability and method for preparation
INVENTOR(S): Mueller, Walter
PATENT ASSIGNEE(S): LTS Lohmann Therapie-Systeme A.-G., Germany
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001039753	A1	20010607	WO 2000-EP11692	20001124
W: AU, BR, CA, CN, CZ, HU, IL, IN, JP, KR, MX, NZ, PL, RU, TR, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 10054713	A1	20010712	DE 2000-10054713	20001104
DE 10054713	C2	20020718		
BR 2000015939	A	20020820	BR 2000-15939	20001124
EP 1233763	A1	20020828	EP 2000-985090	20001124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: DE 1999-19957401 A 19991129
DE 2000-10054713 A 20001104
WO 2000-EP11692 W 20001124

AB The invention concerns transdermal drug delivery systems with increased storage stability that contain carrier and excipient materials of which the sum of the peroxide no. is 20 or less. Ingredients for the drug delivery systems are analyzed; in case of high peroxide no. they can be treated with sulfides to decomp. peroxides, or alternative compns. are explored. Thus two estradiol transdermal systems were prepd. with ingredients: polyacrylate adhesive 16%, glycerin 10%, glycerol ester of partially hydrogenated colophonium 22%, and estradiol 20%. In the first case the peroxide no. of the matrix was 35; in the second case, glycerol ester of partially hydrogenated colophonium was treated with sodium bisulfate, and the peroxide no. decreased to 2-3. Stability studies showed that there were no decompn. products in the second matrix after 6 mo at 25.degree.C and 40.degree.C; but 0.42% and 0.75% .DELTA.9(11)17-.beta.-estradiol was found in the first prepn.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17-diol (17.beta.)-
RL: ADV (Adverse effect, including toxicity); FMU (Formation, unclassified); BIOL (Biological study); FORM (Formation, nonpreparative)
(transdermal drug delivery systems with improved oxidative stability and method for prepn.)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:898420 HCAPLUS
DOCUMENT NUMBER: 134:80974
TITLE: A computationally based identification algorithm for estrogen receptor ligands: Part 2. Evaluation of a hER.alpha. binding affinity model
AUTHOR(S): Mekenyan, O. G.; Kamenska, V.; Schmieder, P. K.; Ankley, G. T.; Bradbury, S. P.

CORPORATE SOURCE: Laboratory of Mathematical Chemistry, Department of Physical Chemistry, Bourgas University "Prof. As. Zlatarov.", Bourgas, 118010, Bulg.
SOURCE: Toxicological Sciences (2000), 58(2), 270-281
CODEN: TOSCF2; ISSN: 1096-6080
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The objective of this study was to evaluate the capability of an expert system described in the previous paper to identify the potential for chems. to act as ligands of mammalian estrogen receptors (ERs). The basis of the expert system was a structure activity relationship (SAR) model, based on relative binding affinity (RBA) values for steroidal and nonsteroidal chems. derived from human ER.alpha. (hER.alpha.) competitive binding assays. The expert system enables categorization of chems. into RBA ranges of <0.1, 0.1 to 1, 1 to 10, 10 to 100, and >150% relative to 17.beta.-estradiol. In the current anal., the algorithm was evaluated with respect to predicting RBAs of chems. assayed with ERs from MCF7 cells, and mouse and rat uterine prepns. The best correspondence between predicted and obsd. RBA ranges was obtained with MCF7 cells. The agreement between predictions from the expert system and data from binding assays with mouse and rat ER(s) were less reliable, esp. for chems. with RBAs less than 10%. Prediction errors often were false positives, i.e., predictions of greater than obsd. RBA values. While discrepancies were likely due, in part, to species-specific variations in ER structure and ligand binding affinity, a systematic bias in structural characteristics of chems. in the hER.alpha. training set, compared to the rodent evaluation data sets, also contributed to prediction errors. False-pos. predictions were typically assocd. with ligands that had shielded electroneg. sites. Ligands with these structural characteristics were not well represented in the training set used to derive the expert system. Inclusion of a shielding criterion into the original expert system significantly increased the accuracy of RBA predictions. With this addnl. structural requirement, 38 of 46 compds. with measured RBA values greater than 10% in hER.alpha., MCF7, and rodent uterine prepns. were correctly categorized. Of the remaining 129 compds. in the combined data sets, RBA values for 65 compds. were correctly predicted, with 47 of the incorrect predictions being false positives. Based upon this exploratory anal., the modeling approach, combined with a high-quality training set of RBA values derived from a diverse set of chem. structures, could provide a credible tool for prioritizing chems. with moderate to high ER binding affinity for subsequent in vitro or in vivo assessments.

IT **791-69-5**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(computationally based identification algorithm for estrogen receptor ligand .alpha. binding affinity)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

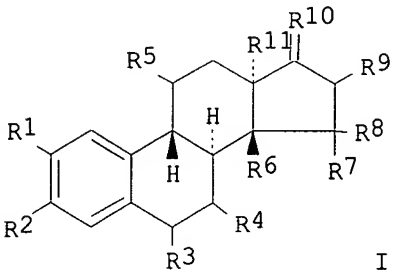
L17 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:738805 HCAPLUS
DOCUMENT NUMBER: 133:296594
TITLE: Preparation of ent-steroids as selectively effective estrogens
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19917930	A1	20001019	DE 1999-19917930	19990415
WO 2000063228	A1	20001026	WO 2000-EP3470	20000417
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1169336	A1	20020109	EP 2000-925219	20000417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002542255	T2	20021210	JP 2000-612318	20000417

PRIORITY APPLN. INFO.: DE 1999-19917930 A 19990415
WO 2000-EP3470 W 20000417

OTHER SOURCE(S): MARPAT 133:296594

GI



I

AB The invention describes new ent-steroids I [R1 = H, OR12, alkenyloxy, alkynyloxy, OSO2R13; R2 = OR12, OSO2R13, OC(:O)R16; R3, R4, R5, R8, R9 = H, halogen, OR12, OSO2R13, R16 ; R6 = .beta.-H; R7 = H; R6R7 = .alpha.-, .beta.-CH2; R10 = H2, dihalogen, H and a halogen, :CR17R18; R11 = H, Me, Et; R12 = H, C1-5-alkyl, C1-5-alkenyl; R13 = , NR14R15; R14, R15 = H, C1-5-alkyl, COR16, C3-7-cycloalky, aryl; R14R15 = polymethylene; NR14R15 = morpholine; R16 = C1-12-alkyl, C1-12-alkenyl, C1-12-alkynyl; R17, R18 = H, halogen, H and OR12, H and OSO2R13, R12 and OC(:O)R16, O; one or more double bonds at C(6)-C(7), C(7)-C(8), C(8)-C(9), C(9)-C(11), C(11)-C(12), C(8)-C(14), C(14)-C(15), C(15)-C(16), C(16)-C(17)], as pharmaceutically active substances, which exhibit in vitro a higher affinity at estrogen receptor of rat prostate than at estrogen receptor of Rat uterus and in vivo a preferential effect at the bone in the comparison to the uterus, their prodn., its therapeutic application and pharmaceutical compns., which contain the new compds. Thus, ent-estriol (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = .beta.-OH, R11 = Me) was prepd. stereoselectively from ent-3,16.alpha.-dihydroxyestra-1,3,5(10)-trien-17-one (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = O, R11 = Me) via redn. with NaBH4 in MeOH. Furthermore the invention describes the use of steroids, those with the (8.alpha.-H,9.beta.-H,10.alpha.-H,13.alpha.-H,14.beta.-H)-gonane skeleton, for the treatment of estrogen deficiency conditioned diseases and conditions.

IT **300853-09-2P**, ent-Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of ent-steroids as selectively effective estrogens)

L17 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:557806 HCAPLUS
DOCUMENT NUMBER: 131:341890
TITLE: Gamma irradiation for terminal sterilization of 17.beta.-estradiol loaded poly(dl-lactide-co-glycolide) microparticles
AUTHOR(S): Mohr, D.; Wolff, M.; Kissel, T.
CORPORATE SOURCE: Schwarz Pharma AG, Monheim, D-40789, Germany
SOURCE: Journal of Controlled Release (1999), 61(1-2), 203-217
CODEN: JCREEC; ISSN: 0168-3659
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 17.beta.-Estradiol-loaded microparticles using poly(dl-lactide-co-glycolide) polymer (PLG) were prepd. by a modified spray-drying method and the effects of .gamma.-irradn. on drug substance, polymer and microparticles were investigated. Irradn. doses ranging from 5.1 to 26.6 kGy were applied using a 60Co-radiation source. 17.beta.-estradiol drug substance showed excellent stability against .gamma.-irradn. in the investigated dose range, whereas microencapsulated estradiol seems to be converted to conjugation products with PLG, and to a lesser extent to the degrdn. product 9,11-dehydroestradiol. The wt.-av. mol. wt. of the PLG polymers decreased with increasing irradn. dose while polydispersity indexes (Mw/Mn) remained nearly unchanged, compatible with a random chain scission mechanism in lactide/glycolide-copolymer degrdn. In vitro drug release studies showed accelerated kinetics with increasing irradn. doses due to dose dependent polymer degrdn. Microbiol. process monitoring showed decreasing bioburden with increasing spraying time, which was successfully further reduced by applying irradn. sterilization. Microencapsulated test spore suspensions of Bacillus pumilus ATCC 27142, the official test specimen for the .gamma.-sterilization process, revealed effective redn. of bioburden, confirming its published D10 value. Thus, these studies demonstrated efficacy of .gamma.-irradn. as terminal sterilization method for poly-(d,l-lactide-co-glycolide) polymer-based drug delivery systems. The sterilization conditions need to be carefully adjusted for the final dosage form.
IT **791-69-5**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(.gamma.-ray irradn. for sterilization of estradiol-loaded poly(lactide-co-glycolide) microparticles)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:489046 HCAPLUS
DOCUMENT NUMBER: 131:286692
TITLE: 17.beta.-hydroxy-11.alpha.-(3'-sulfanylpropyl)oxy-estra-1,3,5(10)-trien-3-yl sulfamate - a novel hapten structure: toward the development of a specific enzyme immunoassay (EIA) for estra-1,3,5(10)-triene-3-yl sulfamates
AUTHOR(S): Schwarz, Sigfrid; Schumacher, Matthias; Ring, Sven; Nanninga, Anita; Weber, Gisela; Thieme, Ina; Undeutsch, Bernd; Elger, Walter
CORPORATE SOURCE: Division of Research and Development, Jenapharm GmbH and Co.KG, Jena, Germany
SOURCE: Steroids (1999), 64(7), 460-471
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title compd. (I) has been synthesized for the use as hapten in the development of a competitive enzyme immunoassay for estrogen sulfamates. The synthesis started from estradiol diacetate (II). Oxyfunctionalization at C-11 to give 11.alpha.-hydroxy steroid (III) was accomplished by hydroboration/alk. hydrogen peroxide oxidn. of the 9(11)-dehydro deriv., which was obtained from compd. II via 9-hydroxylation with dimethyldioxirane. After transformation of III into the allyl ether, the side chain was thio-functionalized at the .omega.-position affording the thioate in two steps. Selective silyl ether deprotection at position 3 followed by sulfamoylation gave the sulfamate, which in turn was demasked at position 17 and treated with sodium borohydride/aluminum chloride to liberate the side chain thiol. Alternatively, I was synthesized via the disulfides. For the prepn. of the immunogen I was coupled to bovine gamma globulin in a two-step procedure using an amine and thiol specific bifunctional crosslinker. The immunization of rabbits resulted in the formation of antibodies which clearly discriminated the sulfamoylated estrogens from the non-esterified estrogens. The use of a biotinylated hapten deriv. as a tracer in combination with a streptavidin-peroxidase-tetramethylbenzidine based detection system allowed the measurement of estradiol 3-sulfamate in the range of about 1 to 1000 pg/well.

IT **791-69-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 17.beta.-hydroxy-11.alpha.-(3'-sulfanylpropyl)oxy-estra-1,3,5(10)-trien-3-yl sulfamate as a specific enzyme immunoassay (EIA) for estra-1,3,5(10)-triene-3-yl sulfamates)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:720945 HCAPLUS
DOCUMENT NUMBER: 130:147999
TITLE: Prediction of liquid chromatographic retention times of steroids by three-dimensional structure descriptors and partial least squares modeling
AUTHOR(S): Nord, L. I.; Fransson, D.; Jacobsson, S. P.
CORPORATE SOURCE: Department of Chemistry, Swedish University of Agricultural Sciences, Uppsala, SE-750 07, Swed.
SOURCE: Chemometrics and Intelligent Laboratory Systems (1998), 44(1,2), 257-269
CODEN: CILSEN; ISSN: 0169-7439
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Prediction of the retention times of steroids in two liq. chromatog. systems, i.e., straight- and reversed-phase, was modeled by different quant. structure-retention relation (QSRR) methods. The 3-dimensional-QSRR descriptors were generated by a process including semiempirical structure optimization, structure alignments, and electronic 3-dimensional field descriptions by the GRID method or by a novel method based on summation of the electronic charges at grid points (Q-field). The compd. data set was split into a calibration set and a test set using the self-organizing feature map (SOFM) technique. The correlation between the mol. descriptors and the retention time of the compds. in the calibration set was established using the partial least squares (PLS) method. Optimal predictive models were generated by a cross-validation procedure. These models were then used to predict the retention times of the compds. in the independent test set. A further check on the validity of the models was obtained by back-projection of the most important variables of the models onto the mol. structure. The predictive capability of variable-reduced models was examd. The various 3-dimensional-QSRR models generated gave for the reversed-phase system Qprediction2 values in the range 0.60-0.79 for the test set, the

corresponding Qprediction2 values for the straight-phase system being in the range 0.42-0.75. In the former case, variable-reduced models resulted in considerably better predictions, although these were not as good as for those models obtained by classical phys.-chem. descriptors.

IT **791-69-5**
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(prediction of liq. chromatog. retention times of steroids by three-dimensional structure descriptors and partial least squares modeling)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:392743 HCAPLUS
DOCUMENT NUMBER: 129:67923
TITLE: Preparation of 9.alpha.-hydroxy-8.alpha.-estra-1,3,5(10)-trienes
INVENTOR(S): Kosemund, Dirk; Schwarz, Sigfrid
PATENT ASSIGNEE(S): Jenapharm G.m.b.H. und Co. K.-G., Germany
SOURCE: Ger., 10 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19723390	C1	19980610	DE 1997-19723390	19970604
EP 882735	A1	19981209	EP 1998-108657	19980513
EP 882735	B1	20000419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 191918	E	20000515	AT 1998-108657	19980513

PRIORITY APPLN. INFO.: DE 1997-19723390 19970604
OTHER SOURCE(S): CASREACT 129:67923; MARPAT 129:67923
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I-IV [R1 = H, alkyl; R2 = Me, Et; R3, R4 = H, (temporarily protected) OH; or R3R4 = O] are prepd. via hydroboration of the corresponding V, resp. and subsequent oxidn. with alk. H2O2. Thus, 3-methoxyestra-1,3,5(10),8-tetraen-17.beta.-ol in 1,2-dimethoxyethane was treated with borane-dimethyl sulfide complex at 23.degree. for 2.5 h followed by treatment with 3N NaOH and 30% H2O2 to give 3-methoxy-8.alpha.-estra-1,3,5(10)-triene-9.alpha.,17.beta.-ol.

IT **791-69-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of hydroxyestratrienes)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:729790 HCAPLUS
DOCUMENT NUMBER: 128:18778
TITLE: Novel estrogens and their radical scavenging effects, iron-chelating, and total antioxidative activities: 17.alpha.-substituted analogs of .DELTA.9(11)-dehydro-

17.beta.-estradiol
AUTHOR(S): Romer, Wolfgang; Oettel, Michael; Menzenbach, Bernd; Droescher, Peter; Schwarz, Sigfrid
CORPORATE SOURCE: Department of Research and Development, Jenapharm GmbH and Co. KG, Jena, D-07745, Germany
SOURCE: Steroids (1997), 62(11), 688-694
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Antioxidant effects of N,N-dimethyl-p-toluidine, p-cresol, and p-(hydroxy)thioanisole 17.alpha.-substituted analogs of 17.beta.-estradiol and their .DELTA.9(11)-dehydro homologs were investigated using four different in vitro models: rat synaptosomal lipid peroxidn. induced by Fenton's reagent, Fe(II)-chelating activities, the formation of superoxide anion radicals, and total antioxidative activity. Whereas the classical estrogen 17.beta.-estradiol as well as selected phenolic compds. was only moderately inhibiting iron-dependent lipid peroxidn. and stimulating total antioxidative activity, besides .DELTA.9(11)-dehydro-17.beta.-estradiol (J 1213), novel estrogens such as C-17-oriented side chain analogs of 17.beta.-estradiol (J 843, J 872, and J 897) and .DELTA.9(11)-dehydro homologs (J 844, J 864, and J 898) directly altered the iron redox chem. and diminished the formation of superoxide anion radicals generated by a xanthine/xanthine oxidase-dependent luminescence reaction to a great extent. These results suggest that definite modifications in the chem. structure of 17.beta.-estradiol, e.g., the introduction of a .DELTA.9(11)-double bond and/or p-cresol as well as p-(hydroxy)thioanisole C-17 substitution, may result in substantial changes in their antioxidant behavior. These compds. may be drug candidates for treating pathologies related to free radical formation.
IT **791-69-5**, J 1213
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(dehydroestradiol analog radical scavenging and iron-chelating and antioxidative activities in relation to structure)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:638466 HCAPLUS
DOCUMENT NUMBER: 127:288310
TITLE: Induction of the Estrogen Specific Mitogenic Response of MCF-7 Cells by Selected Analogs of Estradiol-17.beta.: A 3D QSAR Study
AUTHOR(S): Wiese, Thomas E.; Polin, Lisa A.; Palomino, Eduardo; Brooks, S. C.
CORPORATE SOURCE: Department of Biochemistry, Wayne State University School of Medicine, Detroit, MI, 48201, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(22), 3659-3669
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Analogs of estradiol-17.beta. (E2) have been evaluated for estrogen receptor (ER) binding affinity and mitogenic potential in the human breast cancer cell line MCF-7. These 42 compds. represent subtle modifications of the natural estrogen structure through the placement of hydroxyl, amino, nitro, or iodo groups around the ring system in addn. to, or as replacement of, the 3- and 17.beta.-hydroxyls of E2. The mitogenic activity of the analogs was found to be related to ER binding only to a limited extent. To elucidate structural features that are uniquely responsible for receptor binding affinity or mitogen potential of

estrogens, the three-dimensional quant. structure-activity (QSAR) method Comparative Mol. Field Anal. (CoMFA) was employed. Sep. CoMFA models for receptor binding and cell growth stimulation were optimized through the use of various alignment rules and region step size. Whereas the CoMFA contour plots did outline the shared structural requirements for the two measured biol. properties, specific topol. features in this set of estrogens were delineated that distinguish mitogenic potential from ER binding ability. In particular, steric interference zones which affected growth extend in a band from above the A-ring to position 4 and below, whereas the ER binding steric interference zones are limited to isolated polyhedra in the 1,2 and 4 positions and the .alpha. face of the B-ring. In addn., electroneg. features located around the A-, B-, or C-rings contribute to receptor affinity. However, growth is dependent only on electroneg. and electropos. properties near the 3-position. In a final QSAR model for the mitogenic response, the value of ER binding was included along with structural features as a descriptor in CoMFA. The resulting 3D-QSAR has the most predictive potential of the models in this study and can be considered a prototype model for the general evaluation of a steroidal estrogen's growth stimulating ability in MCF-7 cells. For example, the location of D-ring contours illustrate the model's preference for 17.beta.-hydroxy steroids over the less mitogenic 17.alpha.- and 16.alpha.-hydroxy compds. In addn., the enhanced mitogenic effect of steric bulk in the 11.alpha.-position is also evident. The QSAR studies in this report illustrate the fact that while ER binding may be a required factor of the estrogen dependent growth response in MCF-7 cells, particular structural characteristics, in addn. to those responsible for tight receptor binding, must be present to induce an optimal mitogenic response. Therefore, this report demonstrates that the CoMFA QSAR method can be utilized to characterize structural features of test compds. that account for different types of estrogenic responses.

IT **791-69-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(3D QSAR study of induction of estrogen specific mitogenic response of MCF-7 cells by selected analogs of estradiol)

L17 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:893368 HCAPLUS
DOCUMENT NUMBER: 124:97856
TITLE: Analysis of steroids. Part 47. Estimation of impurity profiles of drugs and related materials, part 13: identification of impurities in estradiol
AUTHOR(S): Goeroeg, Sandor; Brlik, Janos; Csehi, Attila; Halmos, Zsuzsanna; Herenyi, Bulcsu; Horvath, Peter; Dravecz, Ferenc; Bor, Dezsoe
CORPORATE SOURCE: Chemical Works G. Richter Ltd., Budapest, H-1475, Hung.
SOURCE: Analytical Methods & Instrumentation (1995), 2(3), 154-7
CODEN: ANMIEB; ISSN: 1063-5246
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three minor impurities were detected and identified in estradiol bulk material. Estradiol-17-acetate was identified by HPLC and TLC retention matching with an authentic sample. 9(11)-Dehydroestradiol was identified by means of HPLC/diode-array UV spectroscopy. Using mass spectroscopy and HPLC/diode-array UV spectrum the third impurity was identified as 4-chloro deriv. of estradiol. The identification of the impurities was confirmed by synthesizing the proposed structures and doing retention matching.

IT **791-69-5**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of estradiol impurities by HPLC)

L17 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:525485 HCAPLUS
DOCUMENT NUMBER: 121:125485
TITLE: Skeletal conformations and receptor binding of some 9,11-modified estradiols
AUTHOR(S): Palomino, Eduardo; Heeg, Mary Jane; Horwitz, Jerome P.; Polin, L.; Brooks, S. C.
CORPORATE SOURCE: Walker Cancer Research Institute, Wayne State University, Detroit, MI, 48201, USA
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1994), 50(1-2), 75-84
CODEN: JSBBEZ; ISSN: 0960-0760
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect of the modification of the 9-11 positions on the skeletal conformation of estradiol (E2) has been analyzed by x-ray crystallog. and MM2 mol. mechanics. The 11.beta.-hydroxyl and 11-keto analogs of E2 maintained ring conformations which were similar to the natural hormone (E2). Introduction of a double bond at position 9-11 induced a flattening of the entire steroid mol. An 11.alpha.-hydroxyl group brought about significant changes in the alicyclic rings of E2. 9.beta.-Estradiol and 11-keto-9.beta.-estradiol formed ring conformations which were significantly bent from E2 (below the plane of the A-ring). Examn. of the affinity of these C-ring analogs of E2 for the human estrogen receptor has shown extreme variations. A hydroxyl group placed either .alpha. or .beta. at the 11-position yielded ligands with vastly different and reduced affinities for the receptor. The low affinity of 11.alpha.-hydroxyestradiol (1/300th of E2) may be due to the drastic structural change induced in the alicyclic portion of the mol., as well as, to the steric or electrostatic effects of the .alpha.-hydroxyl group upon the receptor protein. An 11.beta.-hydroxyl group diminished the receptor binding to 1/60th that of E2 without alicyclic ring distortions, whereas a 9-11 unsatn. reduced the binding to 1/5th although this steroid displayed a flattening of rings B, C, and D. The 11-keto function, which had little effect on the conformation of the estrogen nucleus, reduced the affinity of this ligand to 1/1000th that of E2. The neg. bend at the C-ring of 11-keto-9.beta.-estradiol and 9.beta.-estradiol prevented these ligands from binding receptor. Some of the obsd. receptor interactions were related to structural alterations in the estrogen ring system induced by modifications on the 9-11 region.
IT **791-69-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation and receptor binding of)

L17 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:198542 HCAPLUS
DOCUMENT NUMBER: 108:198542
TITLE: Estrogen and antiestrogen interaction with estrogen receptor of MCF-7 cells - relationship between processing and estrogenicity
AUTHOR(S): Gyling, M.; Leclercq, G.
CORPORATE SOURCE: Institut Jules Bordet, l'Univ. Libre, Brussels, Belg.
SOURCE: Journal of Steroid Biochemistry (1988), 29(1), 1-8
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Overnight preincubation of MCF-7 cells with 2 .times. 10-10M estradiol (E2) produced a dramatic redn. of their specific [3H]E2 binding capacity. Scatchard plot anal. revealed that this loss of estrogen receptor (ER) concn., usually termed processing, occurred without any modification of binding properties of the unprocessed receptors. Direct measurement of ER gave residual receptor concns. close to those established by binding

assay, indicating that processing involved the loss of at least 1 epitope other than the steroid binding site. Incubation with increasing amts. of E2 (0.1 to 5 .times. 10-10M) resulted in an increasing redn. of binding capacity, indicating that the extent of processing was assocd. with the hormone concn. Steroidal estrogens other than E2 as well as antiestrogens of the triphenylethylene category behaved similarly in this regard, although the latter compds. usually acted only when at higher concns. The processing capacity of a large series of ligands was compared with the corresponding binding affinity for ER as assessed by classical competitive inhibition of [3H]E2 binding in both cytosol and whole cells. For steroidal estrogens, a large spectrum of concordant values was found which correlated with the known uterotropic activity of the compds. However, weak estrogen and antiestrogens of the triphenylethylene category displayed low processing capacities which were in the order of magnitude of the binding affinities established in whole cells; these values were considerably lower than the corresponding values measured in the cytosol. These observations are consistent with the concept that the capacity of a ligand to process ER is related to its agonistic activity. They also support the hypothesis (Stoessel, S.; Leclercq, G. 1986) that assessment of the ability of a ligand to inhibit the binding of [3H]E2 in whole cells provides an est. of its agonistic activity, an est. which can not be established in the corresponding cytosol assay.

IT **791-69-5**
RL: BIOL (Biological study)
(estrogen receptor processing and mammary tumor cells response to, mol. structure in relation to)

L17 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:116021 HCAPLUS
DOCUMENT NUMBER: 106:116021
TITLE: Competitive binding assay for estrogen receptor in monolayer culture: measure of receptor activation potency
AUTHOR(S): Stoessel, S.; Leclercq, G.
CORPORATE SOURCE: Clin. Lab. Cancerol. Mammaire, Univ. Libre Bruxelles, Brussels, 1000, Belg.
SOURCE: Journal of Steroid Biochemistry (1986), 25(5A), 677-82
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English

AB MCF-7 cells were incubated with [3H]estradiol, unlabeled estradiol, and various estrogens or antiestrogens to measure their relative binding affinity (whole-cell assay). Comparison of the values with those previously established on uterine cytosol with a dextran-coated charcoal assay revealed a good parallelism for both steroid and diphenolic diethylstilbesterol based estrogens. On the contrary, in the whole-cell assay, antiestrogens and weak estrogens of the triphenyl- and gem-diphenylethylene categories always displayed low values which were in the order of magnitude found with weak steroid estrogens. This property was not due to a redn. of binding capacity, nor to the presence in some compds. of an ethoxy-aminoalkyl side-chain (source of antiestrogenicity). The present test can provide an est. of the ability of a given compd. to transform the receptor in a form which interacts with genomic sites involved in the regulation of estrogenic-induced products (activation).

IT **791-69-5**
RL: ANST (Analytical study)
(estrogen receptors binding affinity for, of MCF-7 cells, receptor activation potency evaluation in relation to)

L17 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:121429 HCAPLUS
DOCUMENT NUMBER: 100:121429
TITLE: Synthesis of 11-substituted (containing oxygen group)

estradiol

AUTHOR(S): Li, Zhensu; Tan, Jiayi; Ma, Chengyu

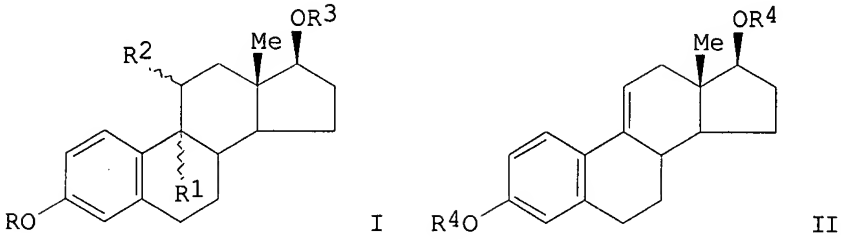
CORPORATE SOURCE: Dep. Pharm. Chem., Beijing Med. Coll., Beijing, Peop. Rep. China

SOURCE: Yaoxue Xuebao (1983), 18(7), 501-6
CODEN: YHHPAL; ISSN: 0513-4870

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



AB Title steroids I (R-R3 = H, .alpha.-H, .alpha.-OH, H; H, .alpha.-H, .beta.-OH, H; H, .alpha.-H, .beta.-MeO, H; H, .beta.-H, .alpha.-MeO, H) were prepd. via a common intermediate I (R-R3 = PhCH2, .alpha.-H, .alpha.-OH, CH2Ph), obtained by benzylation of the estratetraenediol II (R4 = H) and hydroboration-H2O2 oxidn. of II (R4 = PhCH2).

IT **791-69-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of)

L17 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1980:135510 HCAPLUS

DOCUMENT NUMBER: 92:135510

TITLE: Use of borohydride reduction in the separation of estrogen carbonyls

AUTHOR(S): Roos, Robert W.; Medwick, Thomas

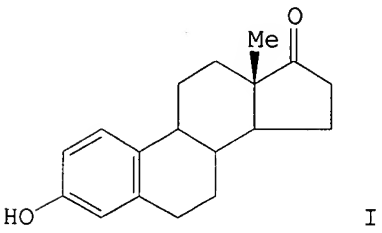
CORPORATE SOURCE: Dep. Health Educ., and Welfare, Food Drug Adm., Brooklyn, NY, 11232, USA

SOURCE: Journal of Chromatographic Science (1979), 17(11), 624-7
CODEN: JCHSBZ; ISSN: 0021-9665

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The chromatog. behavior of the estrogen carbonyls, equilenin [517-09-9], equilin [474-86-2], and estrone (I) [53-16-7] and their resp. NaBH4 redn. products was studied. The sepn. of the 17.beta.-hydroxy reduced

compds. is superior to the sepns. achieved for the parent carbonyls using both reversed-phase and normal-phase systems. The redns. appear quant. by the chromatog. systems used but other work indicates that a small quantity of 17.alpha.-hydroxy isomer is produced. The sepns. developed were used in the identification of 9-dehydroestrone [1089-80-1], an impurity in estrone, and in the identification of the estrogens in a com. aq. suspension of estrogenic substances.

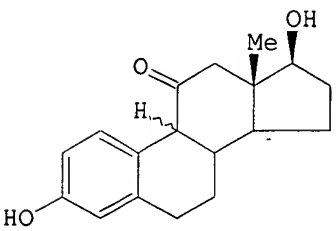
IT **791-69-5**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by high-performance liq. chromatog.)

L17 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1977:406250 HCAPLUS
DOCUMENT NUMBER: 87:6250
TITLE: Oxidation of steroids. IV. The photosensitized oxygenation of 3-keto-17.beta.-hydroxy-5(10)-estrene; steric aspects
AUTHOR(S): Maumy, Michel; Rigaudy, Jean
CORPORATE SOURCE: Ec. Super. Phys. Chim. Ind., Univ. Pierre et Marie Curie, Paris, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1976), (11-12, Pt. 2), 2021-3
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

AB The photosensitized oxygenation of the title compd. I gave 10-hydroperoxy-17.beta.-hydroxyestr-4-en-3-one (II) (.apprx.80%) and the corresponding unstable 10.alpha.-epimer of II, which was not isolated since it readily rearranged to 10,17.beta.-dihydroxy-10.alpha.-estra-1,4-dien-3-one. Refluxing II in toluene for 10 h gave 10,17.beta.-dihydroxyestr-4-en-3-one and 10,17.beta.-dihydroxyestra-1,4-dien-3-one.

IT **63121-72-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L17 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1977:90119 HCAPLUS
DOCUMENT NUMBER: 86:90119
TITLE: Synthesis and conformational stabilities of 11-oxo-9.alpha.- and 9.beta.-estradiol 3-benzyl ether
AUTHOR(S): Liang, C. D.; Baran, J. S.; Allinger, N. L.; Yuh, Y.
CORPORATE SOURCE: Dep. Chem. Res., Searle Lab., Chicago, IL, USA
SOURCE: Tetrahedron (1976), 32(17), 2067-9
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB 11-Oxoestradiol (I; 9.alpha.-H) was prepd., in 50% overall yield, in 5

steps from estradiol via the title ethers. An equilibration study of the 3-benzyl ethers showed that the 9.beta.-epimer is favored over the 9.alpha. by 1.47 kcal/mole. Force field calcns. were carried out for 9.alpha.- and 9.beta.-1,3,5(10)-estratrien-11-one and compared with the exptl. data.

IT **791-69-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(epoxidn. of)

L17 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1976:31287 HCAPLUS
DOCUMENT NUMBER: 84:31287
TITLE: Oxidation of steroids. III. Sensitized photooxygenation of estra-4,9-dien-17.beta.-ol-3-one. Preparation of 9-10 secosteroids and recyclization into new 19-norsteroids
AUTHOR(S): Maumy, Michel; Rigaudy, Jean
CORPORATE SOURCE: Ec. Super. Phys. Chim. Ind., Univ. Pierre et Marie Curie, Paris, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1975), (7-8, Pt. 2), 1879-82
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Hydroperoxyestradiol I, obtined by photooxidn. of estradiene II, underwent acid catalyzed cleavage to give secoestratriene III. Acid catalyzed cyclodehydration of III gave triol IV.
IT **791-69-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and benzylation of)

L17 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1974:75619 HCAPLUS
DOCUMENT NUMBER: 80:75619
TITLE: Application of artificial intelligence for chemical inference. X. INTSUM, a data interpretation and summary program applied to the collected mass spectra of estrogenic steroids
AUTHOR(S): Smith, D. H.; Buchanan, B. G.; White, W. C.; Feigenbaum, E. A.; Lederberg, J.; Djerassi, Carl
CORPORATE SOURCE: Dep. Chem., Stanford Univ., Stanford, CA, USA
SOURCE: Tetrahedron (1973), 29(20), 3117-34
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The INTSUM method was verified using the high resoln. mass spectra of 47 estrogenic steroids and used to examine the fragmentations of equilenins and several acetate and benzoate ester derivs.
IT **791-69-5**
RL: PRP (Properties)
(mass spectroscopy of, computer applications in)

L17 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:537382 HCAPLUS
DOCUMENT NUMBER: 79:137382
TITLE: 11-Alkyl steroids
INVENTOR(S): Baran, John S.; Liang, Chi-Dean
PATENT ASSIGNEE(S): Searle, G. D., and Co.
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3755301	A	19730828	US 1972-265802	19720623
GB 1387960	A	19750319	GB 1973-29512	19730621

PRIORITY APPLN. INFO.: US 1972-265802 19720623
GI For diagram(s), see printed CA Issue.
AB Estratrienediol I was prepd. from estrone (II). Thus, II was dehydrogenated to estratetraenone III, which was treated with NaBH4, Ac2O, and then m-ClC6H4CO2OH to give 9.alpha.,11.alpha.-epoxy-estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol (IV) diacetate. IV diacetate was treated with KOH to give V, which was treated successively with CH2:CHCH2MgBr, SOCl2 and H-Pd/C to yield I. The intermediates had antifertility and estrogenic activity.
IT **791-69-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L17 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:148106 HCAPLUS
DOCUMENT NUMBER: 78:148106
TITLE: Dioxanyl ethers and oxathianyl ethers of natural and synthetic estrogens
AUTHOR(S): Gandolfi, C.; Amendola, M.; Doria, G.; Guidobono, F.; Agresta, G.; Mandelli, V.
CORPORATE SOURCE: Ist. "Carlo Erba" Ric. Ter. S.p.A., Milan, Italy
SOURCE: Farmaco, Edizione Scientifica (1973), 28(3), 186-202
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
AB 1,4-Dioxan-2-yl and 1,4-oxathian-2-yl ethers of steroidal alcs. and phenols were obtained in quant. yield by treating the steroids with 3-4 equivs. of 1,4-diox-2-ene or 1,4-oxathia-2-ene and 3-4 .times. 10-2 equivs. of a sulfonic acid under refux in C6H6. Optically active steroids yielded a 1:1 mixt. of 2 diastereoisomeric ethers, which could be sepd. by fractional crystn. Treatment of estradiol and 17.alpha.-ethynylestradiol with 1,4-diox-2-ene gave the 3,17-bis ethers as a mixt. of 4 diastereoisomers. The 3-monoethers were prepd. indirectly from estrone. Etherification of estradiol 3-benzyl ether, followed by cleavage of the benzyl group by catalytic redn. gave the 17-mono ethers. The 1,4-dioxan-2-yl and 1,4-oxathian-2-yl groups are stable to alkali, but are easily cleaved by acid.
IT **791-69-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 1,4-diox-2-ene and 1,4-oxathia-2-ene)

L17 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:106271 HCAPLUS
DOCUMENT NUMBER: 78:106271
TITLE: Affinity of certain steroids to testosterone-estradiol-binding globulin. II. Androgens
AUTHOR(S): Kuroedova, I. A.; Badanova, Yu. P.; Razmadze, T. G.; Pivnitskii, K. K.; Fanchenko, N. D.
CORPORATE SOURCE: Lab. Biokhim. Endokrinnykh Narushenii, Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR
SOURCE: Problemy Endokrinologii (1973), 19(1), 104-7
CODEN: PROEAS; ISSN: 0375-9660
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Studies of the binding affinity of testosterone (I) [58-22-0], dianabol

[72-63-9], 19-nortestosterone [434-22-0], and several similar steroids, mostly with androgenic activity, to the I-estradiol-binding globulin from human plasma showed that a necessary condition for the interaction is the presence of a free 17.beta.-hydroxyl group to form H-bonds with the globulin. A 17.alpha.-hydroxyl group is sterically incapable of forming these bonds. The B and C rings formed hydrophobic interactions with a nonpolar area of the globulin. Functional groups in position 3 did not affect steroid binding. The C4-C11 segment of the steroid mol. was involved in bonding to the globulin, though less strongly than was the 17.beta.-hydroxyl group.

IT **791-69-5**
RL: PROC (Process)
(globulin binding of)

L17 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:72444 HCAPLUS
DOCUMENT NUMBER: 78:72444
TITLE: 3,17.beta.-Dihydroxy-11.alpha.-methoxyestra-1,3,5(10)-trienes
INVENTOR(S): Pierdet, Andre; Bonne, Claude
PATENT ASSIGNEE(S): Roussel-UCLAF
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2227492	A	19721228	DE 1972-2227492	19720606
DE 2227492	B2	19800228		
DE 2227492	C3	19801016		
FR 2140258	A1	19730119	FR 1971-20453	19710607
IL 39582	A1	19780731	IL 1972-39582	19720531
IL 48282	A1	19780731	IL 1972-48282	19720531
CH 554324	A	19740930	CH 1972-8150	19720601
US 3818056	A	19740618	US 1972-259218	19720602
CA 971559	A1	19750722	CA 1972-143928	19720605
BE 784461	A1	19721206	BE 1972-118333	19720606
NL 7207675	A	19721211	NL 1972-7675	19720606
NL 174047	B	19831116		
NL 174047	C	19840416		
SE 389500	B	19761108	SE 1972-7425	19720606
GB 1389945	A	19750409	GB 1972-26455	19720607
GB 1390175	A	19750409	GB 1974-43397	19720607
DK 131473	B	19750721	DK 1972-2824	19720607
JP 57049560	B4	19821022	JP 1972-56158	19720607
CA 993862	A2	19760727	CA 1975-221864	19750311
SE 7508398	A	19750723	SE 1975-8398	19750723
SE 408897	C	19791025		
SE 408897	B	19790716		

PRIORITY APPLN. INFO.:

FR 1971-20453	19710607
IL 1972-39582	19720531
CA 1972-143928	19720605

GI For diagram(s), see printed CA Issue.

AB Two title compds. (I, X = H, R = Me, R1 = H or C.tplbond.CH), useful as antiestrogenic, antigonadotropic, and antiandrogenic drugs, were prepd. by hydration of the tetraene II with LiAlH4-BF3.Et2O in Et2O and H2O2 treatment in THF, O-methylation with MeI, and hydrogenolytic benzyl ether cleavage optionally followed by ethynylation.

IT **791-69-5**
RL: RCT (Reactant); RACT (Reactant or reagent)

(etherification of)

L17 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:434753 HCAPLUS
DOCUMENT NUMBER: 77:34753
TITLE: Photochemical reactions. 68. Photoisomerization of .alpha.,.beta.-unsaturated .gamma.,.delta.-epoxyketones, 9.alpha., 10.alpha.- and 9.beta., 10.beta.-oxido-3-Oxo-17.beta.-acetoxy-.DELTA.4-estrene
AUTHOR(S): Bauer, D.; Iizuka, T.; Schaffner, K.; Jeger, O.
CORPORATE SOURCE: Org.-Chem. Lab., Eidg. Tech. Hochsch., Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1972), 55(3), 852-73
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Irradn. of 3-oxo-9.alpha.,10.alpha.-epoxy-17.beta.-acetoxyestr-4-ene (I) in EtOH at -65.degree. in the n .fwdarw. .pi.* absorption band gave 3,9-dioxo-17.beta.-acetoxy-8(9 .fwdarw. 10.beta.)-abeoestr-4-ene (II) but gave an identical mixt. of II (major product), 3,9-dioxo-17.beta.-acetoxy-8(9 .fwdarw. 10.alpha.)-abeoestr-4-ene (III), and 3,9-dioxo-17.beta.-acetoxy-11(9 .fwdarw. 10.alpha.)-abeoestr-4-ene (IV) by irradn. at 24.degree. or with triplet sensitization by Michler's ketone and with PhCOMe. Selective .pi. .fwdarw. .pi.* excitation of I at -78.degree. and +24.degree. gave II, III, and IV. 3-Oxo-9.beta., 10.beta.-epoxy-17.beta.-acetoxyestr-4-ene (V) isomerized to III and IV at 24.degree. by n .fwdarw. .pi.* or .pi. .fwdarw. .pi.* excitation. I and V and II-IV were not photochem. interconverted. Photolysis of II-IV gave 3,9-dioxo-17.beta.-acetoxy-8(9 .fwdarw. 10.beta.)abeoestr-5-ene (VI), 3,9-dioxo-17.beta.-acetoxy-8(9 .fwdarw. 10.alpha.)-abeoestr-5-ene and 3,9-dioxo-17.beta.-acetoxy-11(9 .fwdarw. 10.alpha.)-abeoestr-5-ene, resp. Cleavage of II to 3,9-dioxo-17.beta.-acetoxy-.DELTA.4,8(10)-8(9 .fwdarw. 10)-abeo-9,10-seco-estradiene competed with double bond shift, to give VI, when photolyzed in alcs. instead of benzene. The mechanisms of the reactions were discussed.
IT **791-69-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L17 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1971:529996 HCAPLUS
DOCUMENT NUMBER: 75:129996
TITLE: Dehydrogenation of steroids. XVII. Dehydrogenation of estrogens and 3-acetaminoestra-1,3,5(10)-trien-17.beta.-ol with 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ)
AUTHOR(S): Bodenberger, Alfred; Dannenberg, Heinz
CORPORATE SOURCE: Max-Planck-Inst. Biochem., Munich, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1971), 104(8), 2389-404
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The title reaction led to 3-29% of the corresponding 12-oxo-9, 11-dehydro derivs. (I) [where R = OH, OMe, or NHAc; R1 = H or OH; R2 = H or Me; or (R1R2 =)O] and only in the case of 17.beta.-OH substituents, by opening of ring D, an addnl. 28-62% of the corresponding dihydrophenanthhrenes (II) (R = OH, OMe, or NHAc; R3 = CHO or Ac). The acetamido compd. gave an addnl. 2.5% of the corresponding 1,3,5-(10),6,8,14-hexaene. The uv, ir, NMR, and mass spectral data are reported. The estrogenic activities were tested.
IT **791-69-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

L17 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1969:481600 HCAPLUS
DOCUMENT NUMBER: 71:81600
TITLE: Cotton effect of the styrene chromophore
AUTHOR(S): Crabbe, Pierre
CORPORATE SOURCE: Univ. Nac. Auton. Mexico, Mexico, D. F., Mex.
SOURCE: Chemistry & Industry (London, United Kingdom) (1969), (27), 917-18
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The helicity rule for skewed dienes is inverted in the case of styrene chromophore as shown by estratetraenes. All .DELTA.6-estrone derivs. examd. are skewed styrenes with a right-handed helical conformation and exhibit neg. O.R.D. and a circular dichroism curve in the 260-80 nm. region. Conversely, .DELTA.8- and .DELTA.9(11)-steroids with an aromatic A ring show a pos. Cotton effect assocd. with the left-handed helix formed by the styrene chromophore. Another Cotton effect was observed at 230 nm. whose sign and intensity varied with the substitution pattern of the aromatic ring. The largest Cotton effects are assocd. with the 270 nm. transition where the intensity is affected not only by the nature and position of the substituents, but also by the rigidity of the skewed system.
IT **791-69-5**
RL: PROC (Process)
(optical rotatory dispersion of)

L17 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:421007 HCAPLUS
DOCUMENT NUMBER: 65:21007
ORIGINAL REFERENCE NO.: 65:3929f
TITLE: The preparation and chemistry of 9.alpha.,10.alpha.-oxidoestra-4-en-3-ones
AUTHOR(S): Farkas, E.; Owen, J. M.
CORPORATE SOURCE: Lilly Res. Labs., Indianapolis, IN
SOURCE: J. Med. Chem. (1966), 9(4), 510-12
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of estra-4,9(10)-dien-3-ones with peracid affords 9.alpha.,10.alpha.-oxido compds. in high yield. Upon treatment of the oxides with base or acid, .DELTA.9(11)-estradiols or ethers of these diols, resp., are obtained. With pyrrolidine the oxides rearranged to yield 3-pyrrolidinoestra-1,3,5(10)-trien-9.alpha.-ols and 3-pyrrolidinoestra-1,3,5(10),9(11)-tetraenes. The pharmacology of these compds. is summarized.
IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

L17 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1965:9294 HCAPLUS
DOCUMENT NUMBER: 62:9294
ORIGINAL REFERENCE NO.: 62:1714f-h,1715a-b
TITLE: Dehydro-D-homo-C-norestranes
INVENTOR(S): Johns, William F.
PATENT ASSIGNEE(S): G. D. Searle & Co.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3155729		19641103	US	19610213

GI For diagram(s), see printed CA Issue.

AB 17.beta.-Methylestra-1,3,5(10),13-tetraen-3-ol 3-Me ether (I) was converted by ozonolysis or OsO4HIO4 treatment to 3-methoxy-17.beta.-methyl-13,14-seco-18-norestra-1,3,5(10)-triene-13,14-dione (II), cyclized and dehydrated to 3-methoxy-17.beta.-methyl-D-homo-C-norestra-1,3,5(10),13-tetraen-17a-one (III), converted with base to 3-methoxy-17.beta.-methyl-8.alpha.-D-homo-C-norestra-1,3,5(10),13-tetraen-17a-one (IV), and hydrogenated to 3-methoxy-17.beta.-methyl-8.alpha.,13.alpha.,14.alpha.-D-homo-C,18-bisnorestra-1,3,5(10)-trien-17a-one (V). Quantities are expressed in parts by wt. unless otherwise noted. Stirring at room temp. 15 hrs. a mixt. of I 9.4 in Et2O 105 and OsO4 8.9 parts, dilg. with EtOH 320 then 5% aq. Na2SO3 210 parts, refluxing the aq. mixt., 1 hr. filtering, concg. the filtrate, dilg. with H2O, and extg. with 50% EtOAc-C6H6 gave on work-up and chromatography on silica gel with 5% EtOAc in C6H6-elution 17.beta.-methyl-18-norestra-1,3,5(10)-triene-3,13.alpha.,14.alpha.-triol 3-Me ether (VI), m. 126-8.degree. (Me2CO-petr. ether), .lambda. 2.83, 2.99 .mu.. Further elution with 10% EtOAc in C6H6 gave 17.beta.-methyl-18-norestra-1,3,5(10)-triene-3,13.beta.,14.beta.-triol 3-Me ether, m. 136-8.degree. (Me2CO-petr. ether), .lambda. 3.00 .mu.. A mixt. of VI 3.5 in MeOH 400 contg. C5H5N 40 parts added to HIO4 5 in H2O 100 parts was held 22 hrs. at room temp. and dild. with H2O to give II, m. 139-41.degree. (Me2CO-petr. ether), .lambda. 5.86, 5.90 .mu.. Alternatively, passing a stream of O contg. O3 at -70.degree. through a soln. of I 3.1, CH2Cl2 200, and MeOH 40 parts until 0.75 part O3 was introduced over 20 min., adding Zn dust 10 and soln. of HOAc 10.5 in CH2Cl2 13.4 parts, stirring 30 min. with the temp. rising to 5.degree., filtering, washing with aq. KHCO3, working-up, and chromatographing gave II. Stirring 10 min. at room temp. a mixt. of II 1.5 in MeOH 60 and 1% aq. KOH 7.5 parts, and dilg. with H2O, then dil. HCl gave on filtration and chromatography III, m. 140-2.degree. (Me2CO-petr. ether), .lambda. 6.03, 6.19 .mu.; 225, 231, 252 m.mu.. Further elution gave 14.alpha.-hydroxy-3-methoxy-17.beta.-methyl-D-homo-C,18-bisnorestra-1,3,5(10)-trien-17a-one, m. 117-19.degree., .lambda. 2.85, 5.89 .mu.. Refluxing 1 hr. under N a soln. of III 5, MeOH 800, and 5% aq. KOH 100 parts, cooling, and dilg. with H2O gave IV, m. 93-5.degree. (petr. ether), .lambda. 6.00, 61.0, 6.21 .mu.; 227, 250 m.mu.. Hydrogenation to completion of IV 2.6, EtOH 240, and 5% Pd-C 3 parts gave on work-up and chromatography V, m. 88-93.degree., [.alpha.]D 25.degree.. Similar hydrogenation of III gave 3-methoxy-17.beta.-methyl-D-homo-C,18-bisnorestra-1,3,5(10)-trien-17a-one. The 3-Et ether of I was treated as above to give corresponding 3-Et ether compds.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

L17 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1965:3254 HCAPLUS
DOCUMENT NUMBER: 62:3254
ORIGINAL REFERENCE NO.: 62:614f-h
TITLE: .DELTA.9(11)-Dehydroestrone, estradiol, and derivatives
INVENTOR(S): Denot, Ernesto; Bowers, Albert
PATENT ASSIGNEE(S): Syntex Corp.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 3151134 19640929 US 19611003
GI For diagram(s), see printed CA Issue.
AB Estrone 3-Me ether (1 g.) in 15 ml. dioxane and 45 ml. tert-BuOH refluxed 24 hrs. under N with 4 g. chloranil and the residue chromatographed (Al2O3) gave .DELTA.9(11)-dehydroestrone 3-Me ether (I), m. 145-8.degree., [.alpha.]D 299.degree. (CHCl3). I (600 mg.) and 1.5 g. C5H5N.HCl heated 40 min. under N at 200-10.degree. gave .DELTA.9(11)-dehydroestrone, m. 248-51.degree. (MeOH), [.alpha.]D 195.degree. (alc.). The following compds. were similarly prepd.: .DELTA.9(11)-dehydroestradiol, m. 174-5.degree. (aq. Me2 CO), [.alpha.]D 127.degree.; 3,17-diacetate m. 134-5.degree. (MeOH), [.alpha.]D 79.degree.; other related steroids were similarly prepd. but no phys. constants were given. These products had antiandrogenic activity and served as intermediates for the prepn. of 19-norsteroids.
IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

L17 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1964:31241 HCAPLUS
DOCUMENT NUMBER: 60:31241
ORIGINAL REFERENCE NO.: 60:5592d-h,5593a-b
TITLE: Steroid Studies. XLI. Stereochemistry of steroids containing aromatic A-ring. 1. Reactions of 9(11)-dehydroestrone
AUTHOR(S): Tsuda, Kyosuke; Nozoe, Shigeo; Okada, Yutaka
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Chem. Pharm. Bull. (Tokyo) (1963), 11(8), 1022-7
DOCUMENT TYPE: Journal
LANGUAGE: German
AB cf. CA 58, 9164b. Bromination of 9(11)-dehydroestrone Me ether (I) afforded equilenin Me ether (II). Reaction of 9(11)-dehydroestrone acetate (III) with N-bromosuccinimide (IV) provided 3-acetoxy-9.alpha.-hydroxy-11.beta.-bromoestra-1,3,5(10)-trien-17-one (V). Thus, a soln. of 0.145 g. I in 20 ml. CCl4 was treated with a soln. of 0.09 g. Br in 10 ml. CCl4 at 0.degree. to yield 0.05 g. II, m. 191-3.degree. (Et2O). A soln. of 0.15 g. III in 15 ml. CCl4 was treated with 0.08 g. Br in 5 ml. CCl4 at 0.degree. to produce 0.06 g. 3-acetoxy-9.xi.,11.xi.-dibromoestra-1,3,5(10)-trien-17-one (VI), m. 105-6.degree. (decompn.). A soln. of 0.155 g. III in Me2CO contg. 0.125 g. IV was treated with 0.81 ml. 0.2N HClO4 with stirring at 0-3.degree. to produce 0.16 g. V, m. 112-3.degree. (decompn.), [.alpha.]D 220.degree. (all in CHCl3). Treatment of V with Zn-EtOH at 60.degree. for 2 hrs. afforded III. A soln. of 0.33 g. AcOK in 3.3 ml. MeOH was treated with a soln. of 0.406 g. V in 1.55 ml. dioxane at 50.degree., and refluxed 40 min. to give 3-acetoxy-9.alpha.,11.alpha.-epoxyestra-1,3,5(10)-tetraen-17-one (VII), m. 160-2.degree., [.alpha.]D 189.degree.. VII also was prepd. from V by treatment with Zn in EtOH-H2O. A slurry of 0.16 g. V in 5 ml. MeOH was treated with a soln. of 0.053 g. NaOMe in 1 ml. MeOH under N for 15 min. to give 3-hydroxy-9.xi.-estra-1,3,5(10)-triene-11,17-dione (VIII), m. 194-8.degree., [.alpha.]D 244.degree.. VIII also was prepd. by heating 0.1 g. VII in 20 ml. 2.5% KOH in MeOH for 30 min. or by treatment of VII with HCl or CHCl3. A soln. of 5.58 g. III in 20 ml. CHCl3 was treated with 2.96 g. BzOOH in 35.5 ml. CHCl3 24 hrs. to give 5.26 g. VII and 0.07 g. 3-acetoxy-9.beta.,11.beta.-epoxyestra-1,3,5(10)-tetraen-17-one (IX), m. 149-51.degree. (Me2CO-hexane), [.alpha.]D 38.degree.. Redn. of 0.037 g. IX with 0.045 g. LiAlH4 in 4 ml. tetrahydrofuran (THF) provided 9.alpha.-estra-1,3,5(10)-triene-3,11.beta.,17.beta.-triol (X), m. 298-91.degree. (Me2CO). X was also prepd. from the redn. of 11.beta.-hydroxyestrone with LiAlH4. Refluxing 1.15 g. VII with 1.18 g. LiAlH4 in 60 ml. THF 24 hrs. gave 0.6 g. 9.xi.-estra-1,3,5(10)-triene-3,11.alpha.,17.beta.-triol (XI), m. 254-5.degree., [.alpha.]D -52.degree. triacetate m. 127-8.degree. (MeOH), [.alpha.]D -113.degree.. Methylation of 0.39 g. XI in 10 ml. EtOH with 15N NaOH and Me2SO4 gave 0.235 g. the 3-Me ether (XIII), m. 145-6.degree.

(Et2O), [.alpha.]D -58.degree.. A soln. of 0.53 g. V in 14 ml. EtOH was treated with 10 ml. Raney Ni (W-4) in 10 ml. dioxane in the dark at 0-5.degree. for 8 hrs. to give 0.22 g. 3-acetoxy-9.alpha.-hydroxyestra-1,3,5(10)-trien-17-one (XIV), m. 167-8.degree. (Me2CO-hexane), [.alpha.]D 113.degree.. Chromatography of the mother liquor material on SiO2 yielded 0.08 g. XIV and 0.02 g. 3-acetoxyestra-1,3,5(10)-triene-9.alpha.,17.beta.-diol (XV), m. 178-80.degree.. Treatment of 0.2 g. XIV in 2 ml. THF with 0.2 g. LiAlH4 at 0.degree. and then at 25.degree. for 16 hrs. afforded 9(11)-dehydroestradiol (XVI), m. 184-6.degree. (Et2O); diacetate (XVII) m. 148-9.degree. (MeOH), [.alpha.]D 94.degree.. XVII also was prepd. from the redn. of III, followed by acetylation. Redn. of 0.5 g. III with NaBH4 in THF gave 0.44 g. 3-acetoxy-estra-1,3,5(10),9(11)-tetraen-17.beta.-ol (XVIII), m. 123-6.degree.. Treatment of 0.3 g. XVIII with IV at -8 to -5.degree., followed by debromination with Raney Ni provided XV.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

L17 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1963:415891 HCAPLUS
DOCUMENT NUMBER: 59:15891
ORIGINAL REFERENCE NO.: 59:2906b-h,2907a-h,2908a-d
TITLE: 9,11-Disubstituted estratrienes
INVENTOR(S): Reimann, Hans; Robinson, Cecil H.
PATENT ASSIGNEE(S): Schering Corp.
SOURCE: 10 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3076829		19630205	US	19610915

GI For diagram(s), see printed CA Issue.

AB The title products possess estrogenic activity. 9(11)-Dehydroestrone (I) (1 g.) in 5 ml. C5H5N and 0.8 ml. Ac2O left 3 hrs. at room temp. gave 9(11)-dehydroestrone acetate (II), m. 115-17.degree., [.alpha.]D 234.degree. (CHCl3). I (784 mg.) similarly treated with BzCl overnight gave the benzoate (III), m. 232-4.degree., [.alpha.]D 238.degree. (CHCl3). II (250 mg.) and 1 g. LiCl in 12 ml. AcOH stirred 20 min. in the dark with 114 mg. 98% N-chlorosuccinimide and 0.25 ml. 7N HCl gave 9.alpha.,11.beta.-dichloroestrone acetate (IIIa), m. 161-9.degree. (decompn.), [.alpha.]D 13.degree. (CHCl3). II (250 mg.) in 25 ml. dioxane and 2.5 ml. H2O treated 3 hrs. with 150 mg. N-bromosuccinimide and 1 ml. 1.5N HClO4 gave 9.alpha.-bromo-11.beta.-hydroxyestrone acetate (IV). Similarly, I valerate and I caprylate gave the valerate and caprylate esters analogs. 9.alpha.-Bromo-11-oxo-19-nor-4-androstene-3,17-dione with Arthrobacter simplex for 24 hrs. at 28.degree. gave 9.alpha.-bromo-11-oxoestrone. IV (150 mg.) in 10 ml. Me2CO refluxed 17 hrs. with 300 mg. KOAc gave 9.beta.,11.beta.-oxidoestrone acetate (V). The corresponding valerate and caprylate of V were similarly obtained. V was also obtained by treatment of 0.5 g. 9.beta.,11.beta.-oxido-19-nor-4-androstene-3,17-dione with A. simplex followed by acetylation. V (0.5 g.) in 20 ml. CH2Cl2 stirred 3 hrs. in the cold with 2 ml. 48% HF gave 9.alpha.-fluoro-11.beta.-hydroxyestrone 3-acetate. Likewise, V treated with anhyd. HCl 3 min. at -20.degree. gave 9.alpha.-chloro-11.beta.-hydroxyestrone 3-acetate (VI). VI (450 mg.) in 5 ml. AcOH and 1 ml. trifluoroacetic acid anhydride heated 0.5 hr. gave 9.alpha.-fluoro-11.beta.-acetoxyestrone 3-acetate. VI (100 mg.) in 5 ml. Me2CO left 2 hrs. at room temp. with 0.2 ml. CrO3-H2SO4 gave 9.alpha.-fluoro-11-oxoestrone acetate. III (0.5 g.) in 25 ml. CCl4 and 0.4 ml. C5H5N treated at -20.degree. with 0.78 g. Cl in CCl4 stirred 0.5 hr., and warmed to room temp. gave 9.alpha.,11.beta.-dichloroestrone benzoate (VII), m. 136-43.degree. (decompn.), [.alpha.]D 10.1.degree. (dioxane). Similarly,

9.alpha.,11.beta.-dichloroestrone m-toluate was prepd. VII (250 mg.) in 6 ml. Me2SO stirred 10 min. at 20.degree. with 1.5 ml 17% NaC.tplbond.CH in xylene gave 17.alpha.-ethynyl-9.alpha.,11.beta.-dichloroestradiol 3-benzoate (VIIa). I (3 g.) in 300 ml. MeOH left 100 min. with 1 g. NaBH4 gave 9(11)-dehydroestradiol (VIII), m. 191-3.degree.; diacetate (IX) m. 152-3.degree., [.alpha.]D 88.4.degree. (dioxane); dibenzoate (IXa) m. 185-7.degree.. IX (0.5 g.) in dioxane left 2.5 hrs. at room temp. with 210 mg. N-bromoacetamide, 5 ml. H2O, and 2 ml. 1.5N HClO4 gave 9.alpha.-bromo-11.beta.-hydroxyestradiol 3,17-diacetate (X), m. 119-24.degree. (decompn.). The dicaproate and dipropionate esters of I similarly treated gave the corresponding esters of 9.alpha.-bromo-11.beta.-hydroxyestradiol. X (100 mg.) treated with KOAc in Me2CO gave 9.beta.,11.beta.-oxidoestradiol diacetate (XI), m. 122-4.degree.. XI (200 mg.) treated with HF gave 9.alpha.-fluoro-11.beta.-hydroxyestradiol 3,17-diacetate (XIa). VIII (250 mg.) in 25 ml. dioxane stirred 48 hrs. with 100 mg. N-chlorosuccinimide in H2O and 1.5N HClO4 gave 9.alpha.-chloro-11.beta.-hydroxyestradiol 3,17-diacetate (XII). Alternatively, 100 mg. XI treated with anhyd. HCl 2 hrs. in the cold gave XII. IX (354 mg.) in 15 ml. CH2Cl2 and 0.4 ml. C5H5N treated 15 min. at -20.degree. with Cl gave 9.alpha.,11.beta.-dichloroestradiol diacetate (XIIa). 9.alpha.,11.beta.-Dichloroestradiol dicaproate and 9.alpha.11.beta.-dichloroestradiol dipropionate were similarly obtained. IXa with Cl gave 9.alpha.,11.beta.-dichloroestradiol dibenzoate. IX (354 mg.) in 15 ml. CCl4 and 2 ml. C5H5N stirred 20 hrs. with 200 mg. HF in CHCl3-tetrahydrofuran and 146 mg. N-chlorosuccinimide gave 9.alpha.-chloro-11.beta.-fluoroestradiol diacetate. IXa treated with HF and N-chlorosuccinimide as above gave 9.alpha.chloro-11.beta.-fluoroestradiol dibenzoate (XIIb). IX (354 mg.) in Et2CHCO2H stirred 18 hrs. with 152 mg. N-bromoacetamide and 200 mg. HF gave 9.alpha.-bromo-11.beta.-fluoroestradiol diacetate. IX (354 mg.) and 2 g. LiCl in AcOH left 3 hrs. with 152 mg. N-bromoacetamide and HCl gave 9.alpha.-bromo-11.beta.-chloroestradiol diacetate. IX (354 mg.) and 1.5 g. LiOAc treated with 152 mg. N-bromoacetamide gave 9.alpha.-bromo-11.beta.-acetoxyestradiol diacetate. Similarly, IXa gave 9.alpha.-bromo-11.beta.-acetoxyestradiol dibenzoate. IX (354 mg.) in 20 ml. HCO2H contg. 2 g. NaO2CH treated 18 hrs. with N-chlorosuccinimide and HCl gave 9.alpha.chloro-11.beta.-formyloxyestradiol diacetate. 9(11)-Dehydroestrone Me ether (XIII) (282 mg.) in 15 ml. CCl4 and 2 ml. C5H5N treated with 200 mg. HF and 146 mg. N-chlorosuccinimide gave 9.alpha.chloro-11.beta.-fluoroestrone Me ether (XIIIa). Similarly, XIII gave 9.alpha.-bromo-11.beta.-fluoroestrone Me ether, 9.alpha.-bromo-11.beta.-chloroestrone Me ether, and 9.alpha.,11.beta.-dichloroestrone Me ether. XIII (282 mg.) in AcOH treated with N-bromoacetamide and LiAc gave 9.alpha.-bromo-11.beta.-acetoxyestrone Me ether. III (1.5 g.) in 100 ml. tetrahydrofuran treated 1 hr. with NaBH4 gave 9(11)-dehydroestradiol 3-benzoate (XIV), m. 193-4.degree., [.alpha.]D 104.degree. (dioxane). XIV (250 mg.) treated with Cl gave 9.alpha.,11.beta.-dichloroestradiol 3-benzoate (XV). Acetylation of XV gave 9.alpha.,11.beta.-dichloroestradiol 3-benzoate 17-acetate. XIIIa (200 mg.) in Me2SO treated with NaC.tplbond.CH gave 9.alpha.-chloro-11.beta.-fluoro-17.alpha.-ethynylestradiol 3-Me ether. 1,4,9(11)-Androstatriene-3,17-dione (1 g.) in Ac2O heated 5 hrs. with Ac2O and p-MeC6H4SO3H and the resulting acetate hydrolyzed with KOH 20 min. under reflux in H2O gave 1-methyl-9(11)-dehydroestrone (XVI), m. 163-5.degree.. XVI (0.5 g.) treated with Me2SO4 in alkali gave 1-methyl-9(11)-dehydroestrone Me ether (XVIa), m. 100-2.degree., [.alpha.]D 262.degree.. XVI (250 mg.) upon acetylation 22 hrs. gave 1-methyl-9(11)-dehydroestrone acetate (XVII), m. 125-6.degree. [.alpha.]D 215.degree.. XVIa (296 mg.) in 15 ml. CCl4 and 0.4 ml. C5H5N treated with 78 mg. Cl gave 1-methyl-9.alpha.,11.beta.-dichloroestrone Me ether (XVIIa). XVIa similarly afforded 1-methyl-9.alpha.-bromo-11.beta.-fluoroestrone Me ether and 1-methyl-9.alpha.-bromo-11.beta.-chloroestrone Me ether. XVIa (0.5 g.) in dioxane treated with N-bromoacetamide gave 1-methyl-9.alpha.-bromo-11.beta.-hydroxyestrone Me ether.

1-Methyl-9.alpha.-fluoro-11.beta.hydroxyestrone Me ether (XVIIb), and 1-methyl-9.alpha.-chloro-11.beta.hydroxyestrone Me ether were similarly obtained. (XVII) (324 mg.) in CCl4 treated with HF and N-chlorosuccinimide gave 1-methyl-9.alpha.-chloro-11.beta.-fluoroestrone 3-acetate (XVIII). Similarly, XVII treated with N-bromoacetamide gave 1-methyl-9.alpha.bromo-11.beta.-hydroxyestrone 3-acetate (XIX). XIX (200 mg.) in Me2CO heated with KOAc gave 1-methyl-9.beta.,11.beta.-oxidoestrone acetate (XX). XX (100 mg.), treated with HF, gave 1-methyl9.alpha.-fluoro-11.beta.-hydroxyestrone 3-acetate (XXI). XXI (150 mg.) in Me2SO treated with NaC.tplbond.CH gave 1-methyl-9.alpha.-fluoro-11.beta.-hydroxy-17.alpha.-ethynylestradiol 3-acetate. XVI (2.5 g.) in 50 ml. MeOH treated in the cold with 2.5 g. NaBH4 gave 1-methyl-9(11)-dehydroestradiol (XXII), m. 148-52.degree., [.alpha.]D 138.degree.; diacetate (XXIII) m. 128-9.degree., [.alpha.]D 78.degree.. 1-Methyl-9(11)-dehydroestradiol dipropionate (300 mg.) in CCl4 treated with 55 mg. Cl gave 1-methyl-9.alpha.,11.beta.-dichloroestradiol dipropionate. XXIII (200 mg.) treated as above with 80 mg. N-bromoacetamide gave 1 - methyl - 9.alpha. - bromo - 11.beta. - hydroxyestradiol 3,17 - diacetate (XXIIIa). XIII (1 g.) in tetrahydrofuran treated with MeMgI gave 17.alpha.-methyl-9(11)-dehydroestradiol 3-Me ether (XXIV). 17.alpha.-Ethyl-9(11)-dehydroestradiol Me ether was similarly prepd. XVIa similarly treated with MeMgI gave 1,17.alpha.-dimethyl-9(11)dehydroestradiol 3-Me ether (XXIVa). 1-Methyl-17.alpha.-ethyl-9(11)-dehydroestradiol 3-Me ether was similarly prepd. I (2 g.) in tetrahydrofuran treated with MeMgI gave 17.alpha.-methyl-9(11)dehydroestradiol (XXV). Similarly 1,17.alpha.-dimethyl-9(11)-dehydroestradiol was prepd. XXV (1 g.) when acetylated gave 17.alpha.-methyl-9(11)-dehydroestradiol 3-acetate (XXVa). XXIV (298 mg.) in 15 ml. CCl4 and 0.4 ml. C5H5N treated with Cl gave 9.alpha.,11.beta.-dichloro-17.alpha.-methylestradiol 3-Me ether. XXIVa (312 mg.) similarly treated with Cl gave 1,17.alpha.-dimethyl-9.alpha.,11.beta.-dichloroestradiol 3-Me ether. XXIV (500 mg.) in dioxane treated with N-bromoacetamide and HClO4 gave 9.alpha.-bromo-11.beta.-hydroxyestradiol 3-Me ether (XXVI). XXVI (300 mg.) in 20 ml. Me2CO treated with 600 mg. KOAc gave 9.beta.,11.beta.-oxido-17.alpha.methylestradiol 3-Me ether (XXVII). XXVII (0.5 g.) treated with HF in CH2Cl2 gave 9.alpha.-fluoro-11.beta.-hydroxy-17.alpha.-methylestradiol 3-Me ether. 1,17.alpha.-Dimethyl-9.alpha.-fluoro-11.beta.-hydroxyestradiol 3-Me ether was similarly prepd. XXVa treated with HF as above gave 9.alpha.-chloro-11.beta.-fluoro-17.alpha.-methylestradiol 3-acetate. 1,17.alpha.-Dimethyl-9(11)-dehydroestradiol 3-acetate treated with N-bromoacetamide and HClO4 gave 1,17.alpha.-dimethyl-9.alpha.-bromo-11.beta.-hydroxyestradiol 3-acetate. XVIa with N-bromoacetamide and LiOAc gave 1-methyl-9.alpha.-bromo-11.beta.-acetoxy 3-Me ether. XVIIa with NaC.tplbond.CH in Me2SO gave 1-methyl-9.alpha.,11.beta.dichloro-17.alpha.-ethynylestradiol 3-Me ether. XXV (1 g.) in Ac2OC5H5N heated 48 hrs. gave 17.alpha.-methyl-9(11)-dehydroestradiol diacetate (XXVIII). Similarly, acetylation afforded 1,17.alpha.-dimethyl-9(11)-dehydroestradiol diacetate. XXVIII treated with N-bromosuccinimide and HClO4 gave 9.alpha.-bromo-11.beta.-hydroxy-17.alpha.-methylestradiol 3,17-diacetate (XXIX). XXIX with CrO3H2SO4 gave 9.alpha.-bromo-11-oxo-17.alpha.-methylestradiol diacetate (XXX). XXX (1 g.) in 30 ml. 1% K2CO3 and 90% MeOH left 2 hrs. at room temp. gave 9.alpha.-bromo-11-oxo-17.alpha.-methylestradiol 17-acetate. 1,17.alpha.-Dimethyl-9.alpha.-bromo-11-oxoestradiol 17-acetate was similarly prepd. XXIIIa with CrO3 H2SO4 gave 1-methyl-9.alpha.-bromo-11-oxoestradiol diacetate. 9.alpha.-Chloro-11-oxoestradiol diacetate was similarly prepd. and hydrolyzed to the free estradiol (XXXa). XVIIb similarly treated with CrO3-H2SO4 gave 1-methyl-9.alpha.-fluoro-11-oxoestrone 3-Me ether (XXXI). 1-Methyl-9.alpha.-fluoro-11-oxo-17.alpha.-ethynylestradiol 3-Me ether was prepd. from XXXI and NaC.tplbond.CH in Me2SO. 9.alpha.-Fluoro-11-oxo-17.alpha.ethynylestradiol 3-acetate was similarly prepd. XXVa treated with N-bromoacetamide and LiOAc in AcOH gave 9.alpha.-bromo-11.beta.-

acetoxy-17.alpha.-methylestradiol 3-acetate. 1,17.alpha.-Dimethyl-9.alpha.-bromo-11.beta.-acetoxyestradiol 3-Me ether was similarly prepd. XVI with BzCl in C5H5N gave 1-methyl-9(11)-dehydroestrone 3-benzoate (XXXII). XXXII in MeOH with NaBH4 gave 1-methyl-9(11)-dehydroestradiol 3-benzoate (XXXIII). XXXIII with N-bromoacetamide and LiOAc gave 1-methyl-9.alpha.-bromo-11.beta.-acetoxyestradiol 3-benzoate (XXXIV). XIa (200 mg.) in 10 ml. 1% K2CO3 left 1.5 hrs. at room temp. gave 9.alpha.-fluoro-11.beta.-hydroxyestradiol 17-acetate. 1-Methyl-9.alpha.,11.beta.-dichloroestradiol 17-acetate was similarly obtained. XIIb (200 mg.) similarly treated with K2CO3 gave 9.alpha.-chloro-11.beta.-fluoroestradiol 17-benzoate. XXXIV (1 g.) in 10 ml. C6H6N heated 1 hr. with succinic anhydride gave 1-methyl-9.alpha.-bromo-11.beta.-acetoxyestradiol 3-benzoate 17-hemisuccinate. XXXa similarly treated with succinic anhydride gave 9.alpha.-chloro-11-oxoestradiol 3,17-dihemisuccinate (XXXV). XXXV suspended in 100 ml. H2O treated with 10% NaOH gave the 3,17-disodium hemisuccinate. IIIa left overnight with 1% K2CO3 gave 9.alpha.,11.beta.-dichloroestrone (XXXVI). XXXVI (1 g.) and 1 g. pyridine-sulfur trioxide in pyridine stirred 2.5 hrs. at room temp. gave 9.alpha.,11.beta.-dichloroestrone 3-K sulfate (XXXVII). XXXVI (0.5 g.) in 50 ml. H2O brought to pH 7 gave 9.alpha.,11.beta.-dichloroestrone 3-sulfate. XIIa (0.5 g.) similarly left 24 hrs. at room temp. with 20 ml. 1% KOH in MeOH gave 9.alpha.,11.beta.-dichloroestradiol.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

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ACCESSION NUMBER: 1961:38189 HCAPLUS
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TITLE: Steroids. CXVI. CL. 10.beta.-Halo steroids
AUTHOR(S): Mills, J. S.; Barrera, Julia; Olivares, Eugenia; Garcia, Hildelisa
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GI For diagram(s), see printed CA Issue.
AB cf. CA 54, 16478b. The chlorination of steroidal ring A phenols with N-chlorosuccinimide (I) yielded the 10.beta.-chloro-.DELTA.1,4-3-ones (II) in about 25% yield together with a smaller proportion of the 10.beta.,2(or 4)-dichloro-.DELTA.1,4-dien-3-one. Analogous 10.beta.-F dienones (III) were formed on treatment of ring A phenols with perchloryl fluoride (IV) in HCONMe2. Both II and III were readily reducible to the original phenols; however, the III could also be hydrogenated in rather low yields to the satd. 10.beta.-fluoro-5.beta.-3-ketones. The dehydrochlorination of the II gave the .DELTA.9,11-phenols. 10.beta.-Fluoro-.DELTA.1-dehydro-19-nortestosterone (V) readily underwent dienone-phenol rearrangement with Ac2O-H2SO4 to yield the p-fluorophenol diacetate. Estradiol (10 g.) in 400 cc. hot MeCN treated with 7.3 g. I, kept 2 hrs., poured into iced H2O, the product isolated with CH2 Cl2, and chromatographed on 300 g. Al2O3 gave 750 mg. 10.beta.,2(or 4)-dichloro-.DELTA.1-dehydro-19-nortestosterone (VI), m. 183-7.degree. (decompn.), [.alpha.]D -23.degree. (all rotations in CHCl3 unless noted otherwise), and 2.9 g. Cl analog (VII) of V, m. 159-64.degree., [.alpha.]D -6.degree.. Aromatic progesterone (18 g.) in 600 cc. HCONMe2, 40 cc. AcOH, and 40 cc. H2O treated at about 60.degree. with 12.6 g. I, the product isolated with CH2Cl2, and chromatographed on 500 g. Al2O3 yielded 5.05 g. 10.beta.-chloro-.DELTA.1-dehydro-19-norprogesterone (VIII), m. 165-8.degree. (decompn.), [.alpha.]D 77.degree.. 3,17.alpha.-Dihydroxy-17.beta.-acetyl-1,3,5(10)-estratriene (IX) (1 g.) in 40 cc. HCONMe2, 2 cc. AcOH, and 2 cc. H2O heated with 0.65 g. I at about 60.degree. gave 110 mg. 17.alpha.-OH deriv. (X) of VIII.

VI, VII, VIII, and X decompd. in light and more slowly in the dark. IX (4 g.), 1.2 g. p-MeC6H4SO3H, and 50 cc. Ac2O kept at room temp. overnight, poured into H2O, stirred 1 hr., and filtered gave 3.6 g. diacetate (XI), m. 194-5.degree. (MeOH), [.alpha.]D 34.degree.. XI (3.375 g.) in 300 cc. MeOH and 33.75 cc. 1.2% KOH-MeOH kept 10 min. at room temp., treated with 1 cc. AcOH, and concd. yielded 2.79 g. 3,17.alpha.-dihydroxy-17.beta.-acetyl-1,3,5(10)-estratriene 17-monoacetate (XII), m. 242-4.degree. (MeOH), [.alpha.]D 49.degree.. XII (1 g.) in 100 cc. AcOH and 5 cc. H2O and 0.45 g. I heated 2.5 hrs. at 70.degree. yielded 220 mg. 17.alpha.-AcO deriv. (XIII) of VIII, m. 176-8.degree. (decompn.), [.alpha.]D -9.degree.. 17.alpha.-Methylestradiol (XIV) (2 g.) in 40 cc. dioxane and 5 cc. H2O treated with 1.2 g. I and 6 drops 70% HClO4, the mixt. kept at room temp. overnight, worked up and the crude product chromatographed on 60 g. deactivated Al2O3 gave 280 mg. 17.alpha.-Me deriv. hydrate of VIII, needles, m. 75-80.degree. (MeOH), [.alpha.]D -25.degree.. VIII (255 mg.) in 10 cc. 1:1 EtOH-EtOAc hydrogenated 12 min. over 40 mg. Pd-BaCO3 gave 195 mg. 3-hydroxy-17.beta.-acetyl-1,3,5-estratriene, m. 243-7.degree.. VIII (2 g.) and 4 g. CaCO3 in 100 cc. HCONMe2 refluxed 1 hr. under N, filtered through Celite, and poured into H2O pptd. 1.45 g. 3-hydroxy-17.beta.-acetyl-1,3,5(10),9(11)-estratetraene, m. 245-7.degree. (EtOAc), [.alpha.]D 156.degree.; 3-acetate m. 141-2.degree. (MeOH), [.alpha.]D 189.degree.. VIII (1 g.) and 2 g. CaCO3 in 50 cc. HCONMe2 refluxed 1 hr. under N gave 0.82 g. .DELTA.9(11)-dehydroestradiol, m. 174-5.degree. (aq. Me2CO), [.alpha.]D 127.degree.; diacetate m. 134-5.degree. (MeOH), [.alpha.]D 79.degree.. Estradiol (1 g.) in 50 cc. HCONMe2 treated 0.5 hr. with a rapid stream and about 16 hrs. with a very slow stream of IV and poured into dil. aq. NaHCO3, the product isolated with CH2Cl2, and chromatographed on 30 g. Al2O3 yielded V, m. 152-4.degree. (Me2CO-hexane), [.alpha.]D -27.degree.; 17-acetate m. 73.5-75.degree. (hexane), [.alpha.]D -21.degree.. Estrone (10 g.) in 500 cc. HCONMe2 treated 20 hrs. at room temp. with IV gave 7.0 g. 10.beta.-fluoro-19-norandrosta-1,4-diene-3,17-dione, m. 143-4.degree. (Me2CO-hexane), [.alpha.]D 52.degree.. XIV (1 g.) in 500 cc. HCONMe2 with IV yielded 540 mg. 17.alpha.-Me deriv. (XV) of V, m. 100-2.degree. (Me2CO-hexane), [.alpha.]D -52.degree.. 17.alpha.-Ethynylestradiol (1 g.) in 50 cc. HCONMe2 with IV gave 520 mg. 17.alpha.-C.tplbond.CH deriv. of V, m. 160-2.degree. (Me2CO-hexane), [.alpha.]D -80.degree.. 3-Hydroxy-17.beta.-acetyl-1,3,5(10)-estratriene (1 g.) in 50 cc. HCONMe2 gave with IV 660 mg. 10.beta.-F analog of VIII, m. 108-9.5.degree. (Me2CO-hexane), [.alpha.]D 62.degree.. IX (1 g.) in 50 cc. HCONMe2 with IV yielded 630 mg. F analog of X, m. 188-90.degree. (decompn.) (CH2Cl2-MeOH). XII (1 g.) in 50 cc. HCONMe2 with IV yielded 540 mg. F analog of XIII, m. 144-6.degree. (Me2CO-hexane), [.alpha.]D -33.degree.. 3,17.alpha.-Dihydroxy-17.beta.-acetyl-1,3,5(10)-estratriene 3-monoacetate (XVI) (2.54 g.) in 50 cc. CHCl3 treated at room temp. with 58 cc. 2% Br-CHCl3, poured into dil. aq. NaHCO3, and worked up gave 2.55 g. 17.beta.-BrCH2CO analog (XVII) of XVI, m. 161-3.degree. (Me2CO-hexane), [.alpha.]D 56.degree.. XVII (2.48 g.) in 120 cc. MeOH and 3 cc. concd. HCl kept 24 hrs. at room temp. gave 1.99 g. 3,17.alpha.-dihydroxy-17.beta.-bromoacetyl-1,3,5(10)-estratriene (XVIII), m. 181-3.degree. (Me2CO-hexane), [.alpha.]D 81.degree.. XVIII (1.52 g.), 2.2 g. KOAc, and 1.2 g. NaI in 60 cc. Me2CO refluxed 20 hrs. gave 1.03 g. 21-acetate (XIX) of 3,17.alpha.,21-trihydroxy-1,3,5(10)-pregnatrien-20-one (XX), m. 187-90.degree. (Me2CO-hexane), [.alpha.]D 124.degree.. XIX sapond. with KOH-MeOH at 0.degree. gave XX, m. 229-31.degree. (EtOAc), [.alpha.]D 80.degree.. XIX (1 g.) in 50 cc. HCONMe2 with IV yielded 620 mg. 21-acetate (XXI) of 10.beta.-fluoro-17.alpha.,21-dihydroxy-19-norpregna-1,4-diene-3,20-dione (XXII), m. 197-9.degree. (decompn.), [.alpha.]D 49.degree.. XXI hydrolyzed with 10% of its wt. of KOH in MeOH at 0.degree. under N yielded XXII, m. 212-14.degree. (Me2CO), [.alpha.]D 26.degree.. V (500 mg.) in 30 cc. MeOH treated with 1 g. NaBH4 in 4 portions during 1 hr., kept 1 hr. at room temp., and worked up gave 370 mg. estradiol (XXIII), m. 169-71.degree.. V (500 mg.) in 20 cc. MeOH

refluxed 0.5 hr. with excess Raney Ni yielded 405 mg. XXIII, m. 170-2.degree.. .DELTA.1-Dehydroestradiol (910 mg.) in 45 cc. HCONMe2 treated with IV gave 220 mg. 10.beta.-fluoro-.DELTA.1,6-bisdehydro-19-nortestosterone, m. 167-8.degree., [.alpha.]D 60.degree.; 17-acetate m. 127-8.degree. (MeOH), [.alpha.]D 10.degree.. 10.beta.-Fluoro-19-norandrosta-1,4-diene-3,17-dione (2 g.) in 80 cc. EtOH hydrogenated over 1 g. 10% Pd-BaSO4, filtered, evapd., the residue warmed, filtered from 0.9 g. estrone, m. 260.degree., and chromatographed on Al2O3 yielded 150 mg. 10.beta.-fluoro-5.beta., 19-norandrostane-3,17-dione, m. 167-9.degree., [.alpha.]D 98.degree.. V (500 mg.) in 15 cc. C5H5N hydrogenated over 250 mg. 10% Pd-BaSO4 gave 130 mg. 10.beta.-fluoro-17.beta.-hydroxy-5.beta.,19-norandrostan-3-one (XXIV), m. 181-2.5.degree. (Me2CO-hexane), [.alpha.]D 8.degree., and 145 mg. XXIII, m. 168-73.degree.. XV (2.2 g.) in 65 cc. dioxane hydrogenated over 1.1 g. Pd-BaSO4 and the product chromatographed on 66 g. Al2O3 yielded 850 mg. 17.alpha.-Me deriv. (XXV) of XXIV, m. 159-60.degree., [.alpha.]D -12.degree.. Estrololactone (9 g.) in 450 cc. HCONMe2 treated 18 hrs. with IV and the crude product chromatographed on 300 g. Al2O3 yielded 4.18 g. 10.beta.-fluoro-.DELTA.1-dehydro-19-nortestolactone (XXVI), m. 169-71.degree. (Me2CO-hexane), [.alpha.]D -84.degree.. XXVI (1 g.) in 30 cc. dioxane hydrogenated over 500 mg. 10% Pd-BaSO4 and the product chromatographed on 30 g. Al2O3 yielded 450 mg. 10.beta.-fluoro-5.beta.,19-norandrostalacton-3-one (XXVII), m. 195-6.degree. (Me2CO-hexane), [.alpha.]D -39.degree.. 2-Methylestradiol (9 g.) in 450 cc. HCONMe2 treated 20 hrs. with IV and the product chromatographed on 270 g. Al2O3 gave 3.4 g. 2-Me deriv. (XXVIII) of V, m. 173-4.degree. (Me2CO-hexane), [.alpha.]D -51.degree.. XXVIII (2.5 g.) in 80 cc. dioxane hydrogenated over 10% Pd-BaSO4 yielded 1.2 g. 2.beta.-Me deriv. (XXIX) of XXIV, m. 202-4.degree. (Me2CO-hexane), [.alpha.]D 0.5.degree.. XXIX (100 mg.) in 5 cc. 1% KOH-MeOH kept 72 hrs. at room temp. and worked up yielded 98 mg. unchanged XXIX. 2-Methylestrone (22 g.) in 1.5 l. dry tetrahydrofuran treated with 300 cc. 4N EtMgBr, the Et2O distd., the residue refluxed with stirring 3 days, the tetrahydrofuran distd., the residue treated with iced H2O and excess HCl, and the product isolated with CH2Cl2 yielded 15.2 g. 2,17.alpha.-dimethylestradiol (XXX), m. 208-10.degree. (Me2CO-hexane), [.alpha.]D 53.degree. XXX (15 g.) in 750 cc. HCONMe2 treated 18 hrs. with IV and the product chromatographed on 450 g. Al2O3 yielded 7.8 g. 2,1.alpha.-di-Me deriv. (XXXI), m. 176-7.degree. (Me2CO-hexane), [.alpha.]D -64.degree.. XXXI (7.7 g.) in 230 cc. dioxane hydrogenated over 3.75 g. 10% Pd-BaSO4 yielded 3.2 g. 2.beta.-Me deriv. of XXV, m. 92-4.degree. (MeOH), [.alpha.]D -18.degree., and 0.7 g. XXX, m. 199-201.degree.. V (400 mg.), 4 cc. Ac2O, and 3 drops concd. H2SO4 kept 3 hrs. at room temp. gave 360 mg. XXXII (R, R' = OAc), m. 129-32.degree. (CH2Cl2-MeOH), [.alpha.]D 149.degree., which sapond. during 18 hrs. at room temp. with 5% KOH-MeOH yielded XXXII (R, R' = OH), m. 193-4.degree. (Me2CO), [.alpha.]D 183.degree.; this methylated with Me2SO4 and KOH yielded XXXII (R = MeO, R' = OH), m. 119-20.degree. (aq. Me2CO), [.alpha.]D 202.degree.. XXV and XXVII were potent antiandrogens, inhibiting the effect of simultaneously administered testosterone in the rat.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol (prepn. of)

L17 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1959:112030 HCAPLUS
DOCUMENT NUMBER:	53:112030
ORIGINAL REFERENCE NO.:	53:20138h-i,20139a-e
TITLE:	11-Oxygenated estradiol compounds and derivatives
INVENTOR(S):	Hogg, John A.; Korman, Jerome
PATENT ASSIGNEE(S):	Upjohn Co.
SOURCE:	Continuation-in-part of U.S. 2,774,775 (C.A. 51, 6715f)
DOCUMENT TYPE:	Patent
LANGUAGE:	Unavailable

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2885413		19590505	US	

AB 3,11.alpha.,17.beta.-trihydroxy-1,3,5(10)-estratriene (I), m. 250-1.degree., was prepd. by refluxing for 1 hr. 310 mg. 3,11.alpha.-diacetoxy-1,3,5(10)-estratrien-17-one, or the corresponding dihydroxy compd., in 5 ml. C6H6 and 65 ml. Et2O with 0.5 g. LiAlH4, and hydrolyzing with dil. aq. HCl. Recrystn. of 213 mg. of crude solid from MeOH-EtOAc and then from EtOAc gave I. Similarly was obtained 3,11.beta.,17.beta.-trihydroxy-1,3,5(10)-estratriene (II), m. 285-8.degree., [.alpha.]24D 129.degree. (dioxane), from 3,11.beta.-diacetoxy-1,3,5(10)-estratrien-17-one; 3,17.beta.-dihydroxy-1,3,5(10),9(11)-estratetraene (III) from 3-hydroxy-1,3,5(10),9(11)-estratetraen-17-one; 3-methoxy-17.beta.-hydroxy-1,3,5(10),9(11)-estratetraene (IV) from 3-methoxy-1,3,5(10),9(11)-estratetraen-17-one. Catalytic hydrogenation (PtO2) converted III to estradiol and IV to estradiol 3-Me ether. I (520 mg.) in 25 ml. MeOH and 5 ml. H2O contg. 3 g. KOH was cooled to 5.degree. and four 1.5-ml. addns. of (Me2)SO4 were made at 30-min. intervals. MeOH was removed in a stream of air, the residue taken up in CH2Cl2 and chromatographed on 40 g. Florisil. Hexane plus 20% Me2CO eluted 400 mg. (crude) 3-methoxy-11.alpha.,17.beta.dihydroxy-1,3,5(10)-estratriene (V), m. 144-5.degree. (Et2O). In similar fashion was prepd. 3-methoxy-11.beta.,17.beta.-dihydroxy-1,3,5(10)-estratriene from 3,11.beta.,17.beta.-trihydroxy-1,3,5(10)-estratriene. V was also prepd. by LiAlH4 reduction of 3-methoxy-11.alpha.-hydroxy-1,3,5(10)estratrien-17-one. Li (400 mg.) was added to 400 mg. V in 35 ml. anhyd. Et2O and 25 ml. liquid NH3 and cooled in a Dry-Ice Me2CO bath. When the metal dissolved, 4 ml. of abs. EtOH was added during a 30-min. period. The NH3 was then evapd. and H2O added. The oily residue was dissolved in 25 ml. MeOH, 3 ml. H2O, and 1 ml. concd. HCl and refluxed 30 min., and the crude product purified to give 11.alpha.-hydroxy-19-nortestosterone, m. 179-81.degree. (Me2CO). The 11.beta.-hydroxy compd. was converted to 11.beta.-hydroxy-19-nortestosterone in similar fashion. I was converted to 3,11.alpha.,17.beta.-triacetoxy-1,3,5(10)-estratriene by treatment with a large excess of Ac2O in dry C5H5N. The soln. was kept at room temp. 18 hrs. and poured into a mixt. of ice and H2O. The oily product was extd. with CH2Cl2 and purified by chromatography on Florisil using Me2CO-hexane as the eluant. In similar fashion was prepd. 3-methoxy-11.alpha.,17.beta.diacetoxy-1,3,5(10)-estratriene from V; 3;17.beta.-diacetoxy-11.beta.-hydroxy-1,3,5(10)-estratriene (VI) was prepd. in similar fashion by treating II with 2 molar equiv. Ac2O. VI was oxidized to 3,17.beta.-diacetoxy-1,3,5(10)-estratriene-11-one (VII) by means of CrO3 and HOAc and VII hydrolyzed to 3,17.beta.-dihydroxy-1,3,5(10)-estratrien-11-one at room temp. by treatment with NaOMe in MeOH. These compds. exhibit estrogenic activity and are useful intermediates in the prepn. of other estrogenic materials.

IT **791-69-5**, Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
(prepn. of)

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=> fil caold
FILE 'CAOLD' ENTERED AT 19:39:20 ON 22 APR 2003

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

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=> s s l16
MISSING OPERATOR S L16

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L18           7 L16

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L18  ANSWER 1 OF 7  CAOLD  COPYRIGHT 2003 ACS
AN   CA65:3929f  CAOLD
TI   prepn. and chemistry of 9.alpha.,10.alpha.-oxidoestra-4-en-3-ones
AU   Farkas, Eugene; Owen, J. M.
TI   synthesis of natural estradiol methyl ether
AU   Gibian, Heinz; Kieslich, K.; Koch, H. J.; Kosmol, H.; Rufer, C.;
     Schroeder, E.; Voessing, R.
IT    791-69-5    793-53-3   1035-77-4   2162-39-2   4858-90-6
     5720-16-1   5720-17-2   5720-18-3   5720-19-4   6563-75-3   6563-81-1
     6563-82-2   6702-61-0   6733-59-1   6733-79-5   6825-34-9   6854-27-9
     14528-83-7  16215-41-1  24508-05-2

L18  ANSWER 2 OF 7  CAOLD  COPYRIGHT 2003 ACS
AN   CA62:1715b  CAOLD
TI   .DELTA.9(11)-estradiol
AU   Bucourt, Robert; Dube, J.
PA   Roussel-UCLAF
DT   Patent
     PATENT NO.     KIND          DATE
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PI   FR 1370813
IT    791-69-5

L18  ANSWER 3 OF 7  CAOLD  COPYRIGHT 2003 ACS
AN   CA62:614f  CAOLD
TI   .DELTA.9(11)-dehydroestrone, estradiol, and derivs.
AU   Denot, Ernesto; Bowers, A.
PA   Syntex Corp.
DT   Patent
     PATENT NO.     KIND          DATE
     ------------   -----------   ----
PI   US 3151134                   1964
IT    791-69-5    1089-80-1   1670-49-1

L18  ANSWER 4 OF 7  CAOLD  COPYRIGHT 2003 ACS
AN   CA60:5592e  CAOLD
TI   steroid studies - (XLI) stereochemistry of steroids contg. aromatic A ring
     (1) reaction of 9(11)-dehydroestrone
```

AU Tsuda, Kyosuke; Nozoe, S.; Okada, Yutaka
IT **791-69-5** 1089-80-1 1169-54-6 2288-63-3 3907-67-3
5444-22-4 6167-71-1 7627-96-5 94246-54-5 94323-73-6 94544-09-9
94686-56-3 94686-78-9 95720-08-4 95720-11-9 98573-85-4

L18 ANSWER 5 OF 7 CAOLD COPYRIGHT 2003 ACS
AN CA59:2906c CAOLD
TI estratrienes (9,11-disubstituted)
PA Schering Corp.
DT Patent

PATENT NO.	KIND	DATE
US 3076829		1963

IT **791-69-5** 801-53-6 1169-54-6 2070-19-1 2249-42-5
5885-18-7 7291-52-3 15624-35-8 69796-63-0 93947-12-7 95585-34-5
95868-52-3 95870-51-2 96111-90-9 96766-51-7 96972-55-3 97232-22-9
100457-43-0 103673-08-1

L18 ANSWER 6 OF 7 CAOLD COPYRIGHT 2003 ACS
AN CA55:7878h CAOLD
TI creep studies on gelation at 100% relative humidity
AU Eliassaf, J.; Eirich, F. R.
IT **791-69-5**

L18 ANSWER 7 OF 7 CAOLD COPYRIGHT 2003 ACS
AN CA53:20138h CAOLD
TI 11-oxygenated estradiol compds. and derivs.
AU Hogg, John A.; Korman, J.
PA Upjohn Co.
DT Patent

PATENT NO.	KIND	DATE
US 2885413		1959

IT **791-69-5** 2133-53-1 6702-61-0 10516-35-5 14292-07-0
98523-92-3 111089-39-5 111162-56-2 112483-71-3 112571-40-1 114030-49-8

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9
DICTIONARY FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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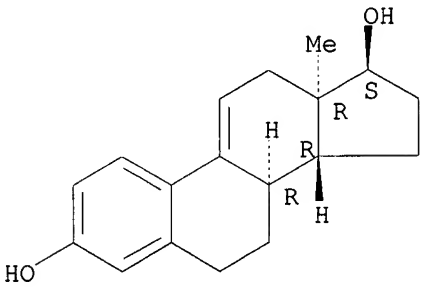
L16 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 428506-98-3 REGISTRY
CN Estra-1,3,5(10),9(11)-tetraene-3,17-diol, (8.alpha.,13.alpha.,14.beta.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN ZYC 12
FS STEREOSEARCH
MF C18 H22 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry. Rotation (-).



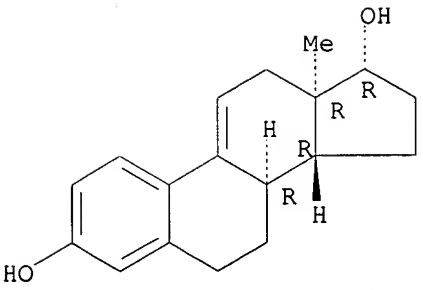
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:386298 this appn.

L16 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 300853-09-2 REGISTRY
CN Estra-1,3,5(10),9(11)-tetraene-3,17-diol, (8.alpha.,13.alpha.,14.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN ent-Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol
CN ZYC 10
FS STEREOSEARCH
MF C18 H22 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:386298 this appn

REFERENCE 2: 133:296594 DE 19917930. 1102(a). a7

L16 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 277329-75-6 REGISTRY
CN Estra-1,3,5(10),9(11)-tetraene-3,17-diol (9CI) (CA INDEX NAME)
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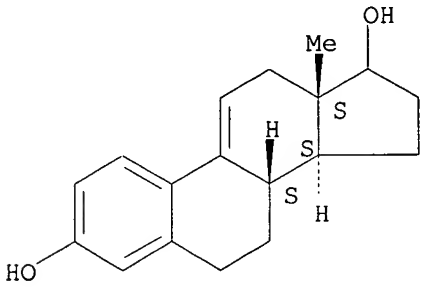
MF C18 H22 O2
SR CAS Registry Services

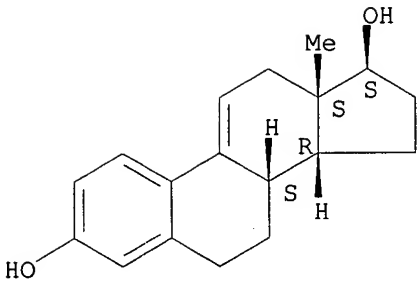
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 63121-72-2 REGISTRY
CN Estra-1,3,5(10),9(11)-tetraene-3,17-diol, (14.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H22 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

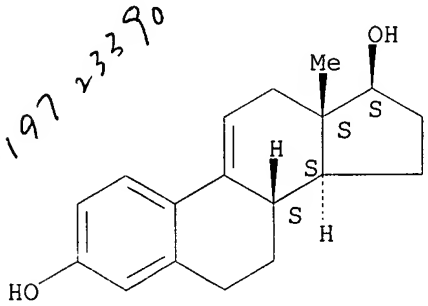
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 87:6250

L16 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 791-69-5 REGISTRY
CN Estra-1,3,5(10),9(11)-tetraene-3,17-diol, (17.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10),9(11)-tetraene-3,17.beta.-diol (6CI, 7CI, 8CI)
OTHER NAMES:
CN .DELTA.9,11-Estradiol
CN 9,11-Dehydroestradiol
CN J 1213
CN ZYC 1
FS STEREOSEARCH
MF C18 H22 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CSCHEM, IFICDB, IFIPAT, IFIUDB, SPECINFO, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

DE 197 23390



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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35 REFERENCES IN FILE CAPLUS (1962 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:50028

REFERENCE 2: 137:140672

REFERENCE 3: 136:386298

REFERENCE 4: 136:161484

REFERENCE 5: 135:10053

REFERENCE 6: 134:80974

REFERENCE 7: 131:341890

REFERENCE 8: 131:286692

REFERENCE 9: 130:147999

REFERENCE 10: 129:67923

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 19:41:54 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 22 Apr 2003  VOL 138 ISS 17
FILE LAST UPDATED: 21 Apr 2003  (20030421/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> d stat que
L1               STR
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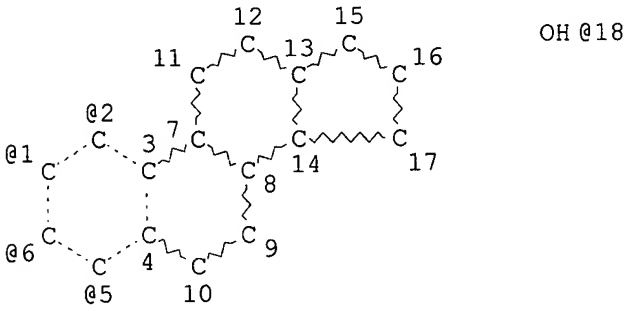


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NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
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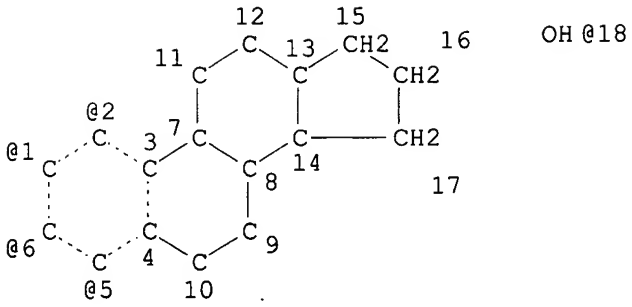

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STEREO ATTRIBUTES: NONE
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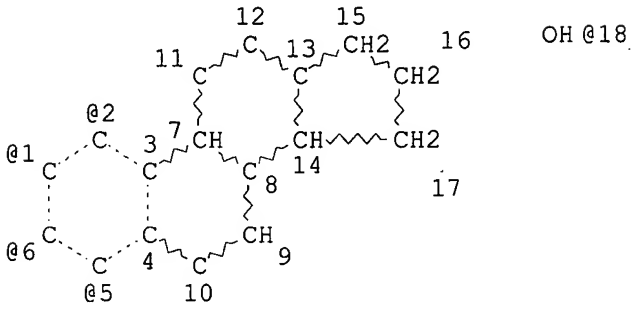

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DEFAULT ECLEVEL IS LIMITED

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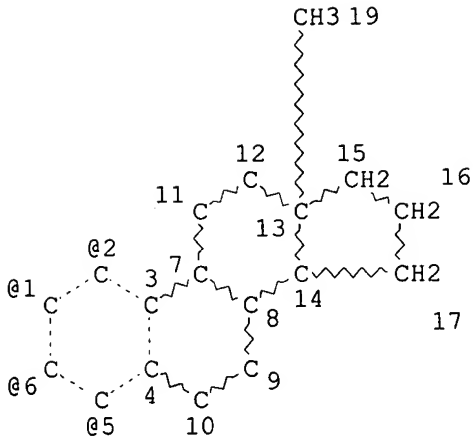
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L6 STR



VPA 18-1/2/5/6 U
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
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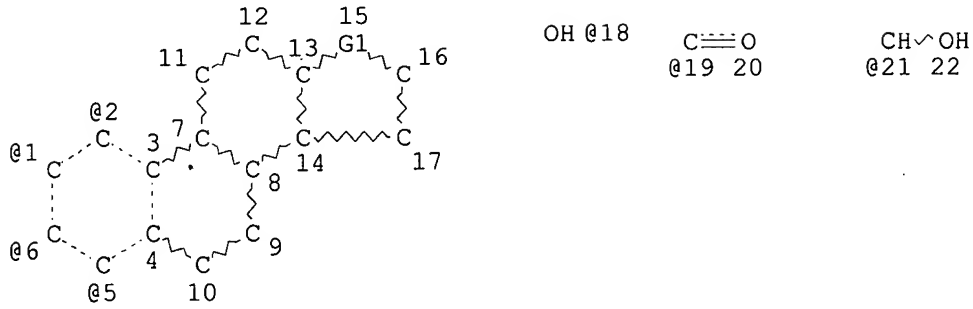

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
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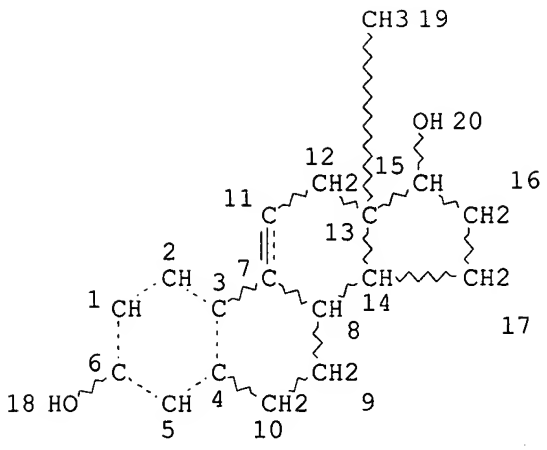
L15 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

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L19        4034 SEA FILE=REGISTRY ABB=ON  PLU=ON  L8 NOT L16
L20        8877 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L21           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)CYTOPROTECT?
L22           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 NOT L17


=>
=>

=> d ibib abs hitrn 122 1-2

L22  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2002:10439  HCAPLUS
DOCUMENT NUMBER:          136:85991
TITLE:                    Preparation of 17.beta.-alkyl ether estradiol
                          derivatives with cytoprotective activity of cells from
                          degeneration through disease, trauma or aging
INVENTOR(S):              Prokai, Laszlo; Simpkins, James W.
PATENT ASSIGNEE(S):       University of Florida Research Foundation, Inc., USA
SOURCE:                   PCT Int. Appl., 29 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
     WO 2002000619      A2   20020103      WO 2001-US41170  20010627
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
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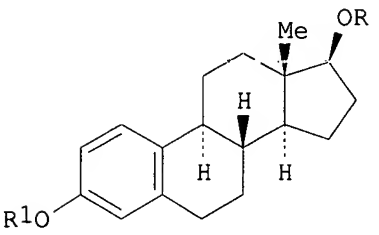
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU,
ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2001077258	A5	20020108	AU 2001-77258	20010627
US 2002035100	A1	20020321	US 2001-893324	20010627
EP 1294446	A2	20030326	EP 2001-955052	20010627

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.:	US 2000-214077P	P	20000627
	WO 2001-US41170	W	20010627

GI



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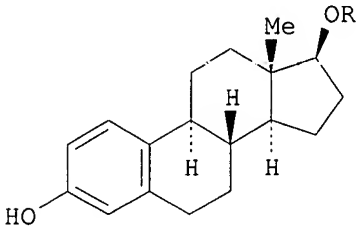

II

AB Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH2)5Me, or (CH2)7Me; R1 = OH) were prepd. in 50-75% yields from 17.beta.-estradiol. 17.beta.-Estradiol and benzyl halide in K2CO3 gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17.beta.-ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepd. in 70 and 75% resp., and were neuroprotective to a similar extent at a concn. of 10 .mu.M and 1 .mu.M. Typical compns. contain approx. 0.01-95% by wt. of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R1 = Bu, (CH2)7Me) were prepd. from 17.beta.-estradiol and Bu or octyl bromide in K2CO3 in 68 and 72% resp.

IT **4954-12-5P 319427-03-7P 319427-04-8P**
319427-06-0P 319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 17.beta.- or 3-alkyl ether derivs. of estradiol used for **cytoprotective** activity of cells from degeneration)

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	2001:114973 HCAPLUS
DOCUMENT NUMBER:	134:158108
TITLE:	Methods of cytoprotection using an enantiomer of estrogen of ischemic damage
INVENTOR(S):	Covey, Douglas F.; Simpkins, James W.
PATENT ASSIGNEE(S):	University of Florida Research Foundation, Inc., USA; Apollo Biopharmaceutics Inc.; Washington University
SOURCE:	PCT Int. Appl., 58 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English

FAMILY ACC. NUM. COUNT: 9
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010430	A2	20010215	WO 2000-US22163	20000811
WO 2001010430	A3	20010830		
WO 2001010430	C2	20020711		
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6350739	B1	20020226	US 1999-372627	19990811
EP 1143947	A2	20011017	EP 2000-957416	20000811
EP 1143947	A3	20020911		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003510336	T2	20030318	JP 2001-526632	20000811

PRIORITY APPLN. INFO.: US 1999-372627 A 19990811
WO 2000-US22163 W 20000811

AB The present invention in various embodiments provides methods of cytoprotection and treatment of disease that include providing an enantiomer of an estrogen compd. to a population of cells in a subject with a cytodegenerative condition to protect those cells from further damage. The enantiomer of the invention is specifically, ent-17.beta.-estradiol or ent-17.beta.-estradiol 17-acetate. Examples of cytodegenerative conditions include stroke and neurodegenerative diseases. The invention further discloses a method of synthesis of ent-17.beta.-estradiol and ent-17.beta.-estradiol 17-acetate. A pharmaceutical formulation comprising an estrogen enantiomer in an oil is also claimed.

IT **300853-33-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(methods of **cytoprotection** using synthetically prepd. estrogen enantiomers)

=>
=> select hit rn l22 1-2
E1 THROUGH E6 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 19:42:19 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9
DICTIONARY FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP

PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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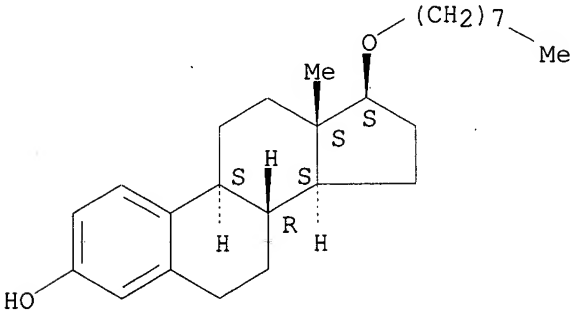
=> s e1-e6
1 300853-33-2/BI
(300853-33-2/RN)
1 319427-03-7/BI
(319427-03-7/RN)
1 319427-04-8/BI
(319427-04-8/RN)
1 319427-06-0/BI
(319427-06-0/RN)
1 319427-07-1/BI
(319427-07-1/RN)
1 4954-12-5/BI
(4954-12-5/RN)
L23 6 (300853-33-2/BI OR 319427-03-7/BI OR 319427-04-8/BI OR 319427-06-0/BI OR 319427-07-1/BI OR 4954-12-5/BI)

=>
=>

=> d ide can l23 1-6

L23 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **319427-07-1** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H40 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

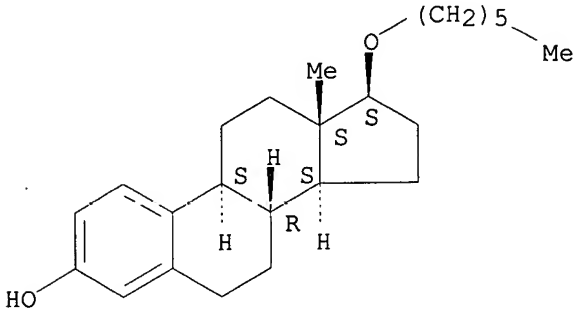
REFERENCE 1: 136:85991

REFERENCE 2: 135:221441

REFERENCE 3: 134:101056

L23 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **319427-06-0** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H36 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

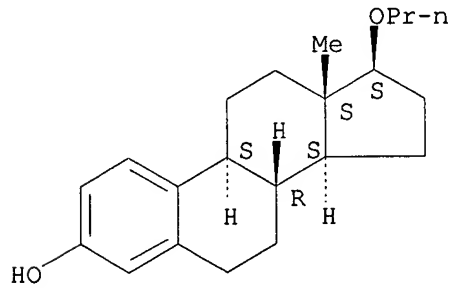
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L23 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **319427-04-8** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H30 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

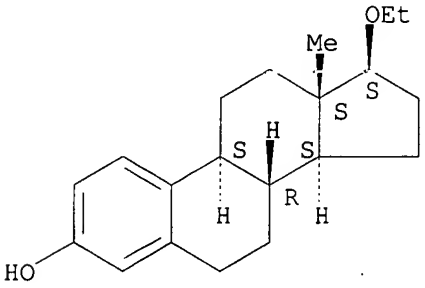
REFERENCE 1: 138:214660

REFERENCE 2: 136:85991

REFERENCE 3: 134:101056

L23 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **319427-03-7** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

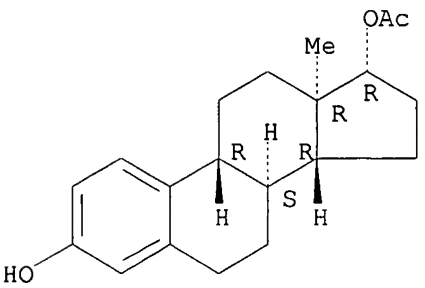
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L23 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **300853-33-2** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 17-acetate,
(8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN ent-Estradiol 17-acetate
FS STEREOSEARCH
MF C20 H26 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:158108

REFERENCE 2: 133:296594

L23 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2003 ACS
RN **4954-12-5** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-3-ol, 17.beta.-methoxy- (7CI, 8CI)
OTHER NAMES:
CN 17-Methoxy-1,3,5(10)-estratrien-3-ol
CN 17.beta.-Methoxyestra-1,3,5(10)-trien-3-ol
FS STEREOSEARCH
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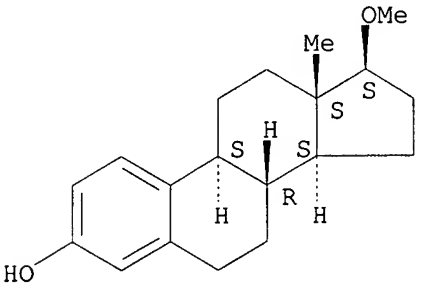
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

19 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
19 REFERENCES IN FILE CAPLUS (1962 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 130:293190

REFERENCE 4: 129:54482

REFERENCE 5: 116:235946

REFERENCE 6: 100:96847

REFERENCE 7: 89:2201

REFERENCE 8: 86:90134

REFERENCE 9: 82:125520

REFERENCE 10: 79:133109

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 19:49:07 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 22 Apr 2003  VOL 138 ISS 17
FILE LAST UPDATED: 21 Apr 2003  (20030421/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L4              STR
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L6              STR
L7              STR
L8         4034 SEA FILE=REGISTRY SUB=L3 SSS FUL L1 NOT (L4 OR L5 OR L6 OR L7)
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L17          37 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16
L19        4034 SEA FILE=REGISTRY ABB=ON  PLU=ON  L8 NOT L16
L20        8877 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L21           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)CYTOPROTECT?
L22           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 NOT L17
L24         357 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L20 AND ?PROTECT?) NOT (L17
                OR L22)
L27         974 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)(?MEDIC? OR ?THERAP? OR
                ?DRUG? OR ?PHARM?)
L29          45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND L27
L30          25 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 NOT (2003 OR 2002 OR
                2001)/PY


=> d ibib abs hitrn l30 1-25

L30  ANSWER 1 OF 25  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2000:880224  HCAPLUS
DOCUMENT NUMBER:          135:71386
TITLE:                    The protective effect of hormone-replacement
                          therapy on fracture risk is modulated by estrogen
                          receptor .alpha. genotype in early postmenopausal
                          women
AUTHOR(S):                Salmen, Timo; Heikkinen, Anna-Mari; Mahonen, Anitta;
                          Kroger, Heikki; Komulainen, Marja; Saarikoski, Seppo;
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Honkanen, Risto; Maenpaa, Pekka H.
CORPORATE SOURCE: Department of Biochemistry, University of Kuopio, Kuopio, Finland
SOURCE: Journal of Bone and Mineral Research (2000), 15(12), 2479-2486
CODEN: JBMREJ; ISSN: 0884-0431
PUBLISHER: American Society for Bone and Mineral Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Genetic factors regulate bone mineral d. (BMD) and possibly development of osteoporosis. It has been suggested that estrogen receptor .alpha. (ER.alpha.) genotype is assocd. with BMD, but the assocn. between ER.alpha. genotype, fracture risk, and postmenopausal hormone replacement therapy (HRT) has not been studied. Therefore, we evaluated whether ER.alpha. polymorphism is assocd. with fracture risk in a 5-yr trial with HRT in a population-based, randomized group of 331 early postmenopausal women. The participants consisted of two treatment groups: the HRT group (n = 151) received a sequential combination of 2 mg of estradiol valerate (E2 Val) and 1 mg of cyproterone acetate with or without vitamin D3, 100-300 IU + 93 mg calcium as lactate per day; and the non-HRT group (n = 180) received 93 mg of calcium alone or in combination with vitamin D3, 100-300 IU/day. All new symptomatic, radiog. defined fractures were recorded. Pvu II restriction fragment length polymorphism of the ER.alpha. was detd. using polymerase chain reaction (PCR). In all, 28 women sustained 33 fractures during the approx. 5.1-yr follow-up. In the HRT group, the ER.alpha. genotype (PP, Pp, and pp) was not significantly assocd. with fracture risk (p = 0.138; Cox proportional hazards model). When the genotypes was dichotomized (PP + Pp vs. pp), the incidence of new fractures in the HRT group was significantly reduced in women with the P allele (p = 0.046) with the relative risk (HR) of 0.25 (95% CI, 0.07-0.98), in comparison with the non-P allele group. After adjustment for time since menopause and previous fracture, the assocn. between the dichotomous genotype and fracture risk persisted with HR of 0.24 (95% CI, 0.06-0.95; p = 0.042). In the non-HRT group, the ER.alpha. genotype was not significantly assocd. with fracture risk. During HRT, women with the pp genotype have a greater fracture risk than those with the P allele. The results suggest that the pp genotype is a relatively hormone-insensitive genotype, and it appears that women with the P allele may benefit more from the **protective** effect of HRT on fracture risk than women with the pp genotype.

IT **979-32-8**, Estradiol valerate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**protective** effect of hormone-replacement **therapy** on fracture risk is modulated by estrogen receptor .alpha. genotype in early postmenopausal women)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:763381 HCAPLUS
DOCUMENT NUMBER: 134:83831
TITLE: Expression of members of the multidrug resistance protein family in human term placenta
AUTHOR(S): St-Pierre, M. V.; Serrano, M. A.; Macias, R. I. R.; Dubs, U.; Hoechli, M.; Lauper, U.; Meier, P. J.; Marin, J. J. G.
CORPORATE SOURCE: Division of Clinical Pharmacology and Toxicology, Department of Internal Medicine, University Hospital, University of Zurich, Zurich, CH-8091, Switz.
SOURCE: American Journal of Physiology (2000), 279(4, Pt. 2), R1495-R1503

CODEN: AJPHAP; ISSN: 0002-9513
PUBLISHER: American Physiological Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The placenta serves, in part, as a barrier to exclude noxious substances from the fetus. In humans, a single-layered syncytium of polarized trophoblast cells and the fetal capillary endothelium sep. the maternal and fetal circulations. P-glycoprotein is present in the syncytiotrophoblast throughout gestation, consistent with a **protective** role that limits exposure of the fetus to hydrophobic and cationic xenobiotics. We have examd. whether members of the multidrug resistance protein (MRP) family are expressed in term placenta. After screening a placenta cDNA library, partial clones of MRP1, MRP2, and MRP3 were identified. Immunofluorescence and immunoblotting studies demonstrated that MRP2 was localized to the apical syncytiotrophoblast membrane. MRP1 and MRP3 were predominantly expressed in blood vessel endothelial with some evidence for expression in the apical syncytiotrophoblast. ATP-dependent transport of the anionic substrates dinitrophenyl-glutathione and estradiol-17-.beta.-glucuronide was also demonstrated in apical syncytiotrophoblast membranes. Given the cellular distribution of these transporters, we hypothesize that MRP isoforms serve to **protect** fetal blood from entry of org. anions and to promote the excretion of glutathione/glucuronide metabolites in the maternal circulation.
IT **1806-98-0**, Estradiol-17.beta.-glucuronide
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(model substrate transport; expression of members of the **multidrug** resistance protein (MRP1-3) family in human term placenta)
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:551045 HCAPLUS
DOCUMENT NUMBER: 133:276521
TITLE: Effect of estrogen-progestin replacement therapy on plasma lipids and lipoproteins in postmenopausal women
AUTHOR(S): Rodriguez-Aleman, F.; Torres, J. M.; Cuadros, J. L.; Ruiz, E.; Ortega, E.
CORPORATE SOURCE: Department of Clinical Biochemistry, S. Cecilio University Hospital, Granada, 18012, Spain
SOURCE: Endocrine Research (2000), 26(2), 263-273
CODEN: ENRSE8; ISSN: 0743-5800
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Serum levels of cholesterol (Chol), triglycerides (TG), low-d. lipoprotein cholesterol (LDL) high-d. lipoprotein cholesterol (HDL), both apolipoproteins A1 and B (Apo A1, Apo B), FSH LH, estradiol (E2), progesterone (P), testosterone (T) and steroid hormone binding globulin (SHBG) were measured in postmenopausal women, before and after four different estrogen-progestin replacement therapies. Each woman was her own control to avoid genetic or socioeconomic differences. The authors' results showed that serum E2 and TG significantly increased and serum FSH, LH, LDH, Apo B, and Chol significantly decreased after all treatments. Serum P and T did not significantly change after any of the treatments. HDL, Apo A1 and SHBG significantly increased in the groups treated with medroxyprogesterone acetate (MPA) but not in the group treated with Norgestrel. The authors conclude that estrogen-progestin replacement therapy in postmenopausal women leads to profound and beneficial changes in plasma lipids and lipoproteins and that treatments with cyclic or continuous MPA could provide greater **protection** against coronary

heart disease (CHD).
IT **979-32-8**, Estradiol valerate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(estrogen-progestin replacement **therapy** effect on plasma lipids and lipoproteins and sex hormones in postmenopausal women)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:7995 HCAPLUS
DOCUMENT NUMBER: 132:217271
TITLE: A randomized trial of oral contraceptive and hormone replacement therapy on bone mineral density and coronary heart disease risk factors in postmenopausal women
AUTHOR(S): Taechakraichana, N.; Limpaphayom, K.; Ninlagarn, T.; Panyakhamlerd, K.; Chaikittisilpa, S.; Dusitsin, N.
CORPORATE SOURCE: Faculty of Medicine, Department of Obstetrics and Gynecology, Chulalongkorn University, Bangkok, Thailand
SOURCE: Obstetrics & Gynecology (New York) (2000), 95(1), 87-94
CODEN: OBGNAS; ISSN: 0029-7844
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Studies were carried out to identify the effects of oral contraceptive (OC) and hormone replacement therapy (HRT) on bone mineral d. and coronary heart disease risk factors in postmenopausal women. Eighty healthy postmenopausal women were randomly assigned to a cyclic regimen of OC contg. 30 .mu.g of ethinyl estradiol and 150 .mu.g of desogestrel or HRT contg. 625 mg of conjugated equine estrogens 21 days per cycle and 5 mg of medrogestone 10 days per cycle for 12 mo. Bone mineral d. of lumbar spine and hip, biochem. markers of bone turnover, lipid-lipoprotein profiles, coagulation profiles, fasting plasma glucose, and blood pressure were evaluated. Both regimens caused significant increase in bone mineral d. of lumbar spine, trochanter, intertrochanteric region, total hip, and Ward triangle. Only OC therapy was assocd. with a significant increase in femoral neck bone mineral d. (mean score .+-. std. error 2.5% .+-. 0.7%). Biochem. markers of bone turnover, total cholesterol, and low-d. lipoprotein cholesterol decreased significantly in both groups. Posttreatment levels of those bone markers and lipid-lipoprotein were significantly lower after OC therapy than HRT. Fasting plasma glucose and systolic blood pressure decreased significantly in both groups; however, only the OC group showed a significant decrease in diastolic blood pressure. Both OC and HRT increased bone mineral d. of lumbar spine and hip, but OC suppressed bone turnover more than HRT. Both methods favorably affected lipid-lipoprotein metab., fasting plasma glucose, and blood pressure during the 12 mo of treatment.
IT **71138-35-7**, Ethinylestradiol-desogestrel mixt.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(oral contraceptive and hormone replacement **therapy** effect on bone mineral d. and coronary heart disease risk factors in postmenopausal women)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:317382 HCAPLUS

DOCUMENT NUMBER: 130:347606
TITLE: Hormone replacement therapy and circulating ICAM-1 in postmenopausal women. A randomised controlled trial
AUTHOR(S): Scarabin, Pierre-Yves; Alhenc-Gelas, Martine; Oger, Emmanuel; Plu-Bureau, Genevieve
CORPORATE SOURCE: Cardiovascular Epidemiology Unit U258, Hopital Broussais, Villejuif, F-94807, Fr.
SOURCE: Thrombosis and Haemostasis (1999), 81(5), 673-675
CODEN: THHADQ; ISSN: 0340-6245
PUBLISHER: F. K. Schattauer Verlagsgesellschaft mbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hormone replacement therapy may reduce the risk of coronary heart disease but underlying mechanism was not adequately explained. Recent data suggest that intercellular adhesion mol. 1 (ICAM-1) plays a crit. role in early stage of atherosclerosis and may serve as a mol. marker for the development of arterial disease. The effects were investigated of oral and transdermal cyclic estradiol combined with progesterone on blood plasma concn. of sol. ICAM-1 (sICAM-1). 37 Healthy postmenopausal women were randomly assigned to receive either oral estradiol valerate or transdermal estradiol both combined with micronized progesterone or no hormonal treatment. Plasma sICAM-1 was assayed at baseline and after a 6-mo period. Oral but not transdermal estradiol regimen decreased mean value of sICAM-1 compared with no treatment. Differences in sICAM-1 levels between active treatments were significant. There were no changes in mean values of fibrinogen between the 3 groups. The results show a favorable effect of oral estrogen plus progesterone on a sol. marker of vascular inflammation and may provide plausible explanation for a **cardioprotective** effect of hormone replacement therapy among healthy postmenopausal women.
IT **979-32-8**, Estradiol valerate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hormone replacement **therapy** and circulating ICAM-1 in postmenopausal women)
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 6 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:43842 HCAPLUS
DOCUMENT NUMBER: 130:105471
TITLE: Effects of add-back therapy on bone mineral density and pyridinium crosslinks in patients with endometriosis treated with gonadotropin-releasing hormone agonists
AUTHOR(S): Gnoth, Christian; Goedtke, Katrin; Freundl, Guenter; Godehardt, Eberhardt; Kienle, Erika
CORPORATE SOURCE: Dep. Gynecology Obstetrics, Academic Hospital, Univ. Duesseldorf, Duesseldorf, D-40593, Germany
SOURCE: Gynecologic and Obstetric Investigation (1999), 47(1), 37-41
CODEN: GOBIDS; ISSN: 0378-7346
PUBLISHER: S. Karger AG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Patients with endometriosis were given gonadotropin-releasing hormone agonists (GnRHa) with or without hormone add-back therapy (+ 20 .mu.g of ethinyl estradiol with 0.15 mg desogestrel) designed to suppress the adverse effects of hypoestrogenism while preserving the efficacy of GnRHa. Both regimens showed improvements in endometriosis, dysmenorrhea, and pelvic pain. Effects were better in the GnRHa + placebo group. The GnRHa + placebo group had higher serum Ca levels and a higher loss of lumbar

spine bone mineral d. (BMD). Urinary levels of pyridinium crosslinks increased in the GnRHa + placebo group, and declined to normal in the GnRHa + add-back group. The add-back therapy **protects** women taking GnRHas from severe loss of BMD and accelerated bone collagen resorption, but reduces the efficacy of the GnRHa.

IT **57-63-6**, Ethinyl estradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(gonadotropin-releasing hormone agonists add-back **therapy** effect on bone mineral d. and pyridinium crosslinks in endometriosis)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:755795 HCAPLUS
DOCUMENT NUMBER: 130:148844
TITLE: The effect of hormone replacement therapy on carotid arteries: measurement with a high frequency ultrasound system
AUTHOR(S): Sator, Michael O.; Joura, Elmar A.; Gruber, Doris M.; Wieser, Fritz; Jirecek, Stefan; Tschugguel, Walter; Huber, Johannes C.
CORPORATE SOURCE: Department of Obstetrics and Gynecology, Division of Gynecological, University Hospital of Vienna, Medical School, Vienna, A-1090, Austria
SOURCE: Maturitas (1998), 30(1), 63-68
CODEN: MATUDK; ISSN: 0378-5122
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Objective: To evaluate the effect of hormone replacement therapy (HRT) on carotid arteries in postmenopausal women with a high frequency ultrasound system. Methods: In a clin. cross-sectional study carotid artery layers were measured in 82 postmenopausal women receiving a sequential regimen of HRT (estradiol valerate 2 mg and dydrogesterone 10 mg) and in 70 postmenopausal women without HRT. Measurements of the left carotid artery layers (externa, media, intima) were taken with a single mech. activated 22.5-MHz transducer with an effective band width of 8 MHz. Results: A statistically significant increase in thickness of the media layer of the carotid artery was obsd. in the HRT group (0.34 mm) as compared to the untreated group (0.27 mm). The media/intima ratio of the treated group was statistically significantly higher than that of the untreated group. The mean strength of the carotid wall was 0.70 mm in the 70 postmenopausal women without HRT and 0.76 mm in the 82 patients undergoing HRT. Conclusion: HRT has a morphol. effect on the carotid arteries in postmenopausal women. These findings support a **cardioprotective** effect, esp. in terms of prevention of atherosclerosis. This effect can be measured non-invasively by high frequency ultrasound.

IT **979-32-8**, Progynova
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hormone replacement **therapy** effect on carotid arteries in postmenopausal women)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 8 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:426576 HCAPLUS
DOCUMENT NUMBER: 129:170691
TITLE: Postmenopausal hormone replacement therapy and autoantibodies against oxidized LDL

AUTHOR(S): Heikkinen, Anna-Mari; Niskanen, Leo; Yla-Herttuala, Seppo; Luoma, Jukka; Tuppurainen, Marjo T.; Komulainen, Marja; Saarikoski, Seppo
CORPORATE SOURCE: Departments of Obstetrics and Gynecology, Kuopio, 70211, Finland
SOURCE: Maturitas (1998), 29(2), 155-161
CODEN: MATUDK; ISSN: 0378-5122
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

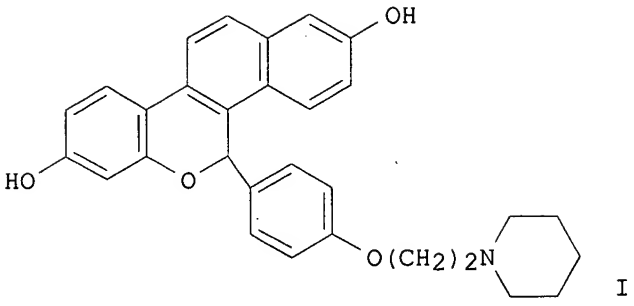
AB Oxidative modification of low-d. lipoprotein (oxLDL) has been suggested to play an important role in the pathogenesis of atherosclerosis, and autoantibodies against oxLDL have recently found to reflect this process. The antioxidant effect and inhibition of LDL oxidn. may be one of the **cardioprotective** mechanisms of postmenopausal estrogen therapy. The effects of postmenopausal hormone replacement therapy (HRT) on the concns. of serum lipids and oxLDL autoantibodies were studied in a population-based prospective 1-yr study with 64 early postmenopausal women (mean age 52.2.+-.0.4 (S.E.M.) years). The participants were randomized into two treatment groups: HRT-group: Sequential combination of 2 mg estradiol valerate and 1 mg cyproterone acetate alone or in combination with vitamin D3, 300 IU/day + calcium lactate, 500 mg/day (n = 31) and the non-HRT-group: Calcium lactate, 500 mg/day alone or in combination with vitamin D3, 300 IU/day (n = 33). The groups were well matched regarding age, body mass index and baseline serum lipid concns. The serum concns. of total cholesterol and LDL-cholesterol decreased in the HRT-group (4.1%, P = 0.05 and 6.4%, P = 0.03, resp., paired t-test) but did not change in the non-HRT-group. No changes in the serum concns. of HDL-cholesterol or triglycerides were obsd. Addnl., no changes in oxLDL autoantibody concns. were obsd. in either group. Although 1-yr HRT lowered serum total- and LDL-cholesterol levels, it did not influence oxLDL antibody titers. On the basis of the present results we cannot question the possibility of there being beneficial effects of HRT on the oxidative modification of LDL. However, this effect is not reflected in the levels of oxLDL autoantibodies.

IT **979-32-8**, Estradiol valerate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(oxidized LDL autoantibodies in women on postmenopausal hormone replacement **therapy**)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:215077 HCAPLUS
DOCUMENT NUMBER: 128:266187
TITLE: Synthesis and Pharmacology of Conformationally Restricted Raloxifene Analogs: Highly Potent Selective Estrogen Receptor Modulators
AUTHOR(S): Grese, Timothy A.; Pennington, Lewis D.; Sluka, James P.; Adrian, M. Dee; Cole, Harlan W.; Fuson, Tina R.; Magee, David E.; Phillips, D. Lynn; Rowley, Ellen R.; Shetler, Pamela K.; Short, Lorri L.; Venugopalan, Murali; Yang, Na N.; Sato, Masahiko; Glasebrook, Andrew L.; Bryant, Henry U.
CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(8), 1272-1283
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
GI



I

AB Raloxifene is a selective estrogen receptor modulator (SERM) which is currently under clin. evaluation for the prevention and treatment of postmenopausal osteoporosis. In vivo structure-activity relationships and mol. modeling studies indicated that the orientation of the basic amine-contg. side chain of raloxifene relative to the stilbene plane is an important discriminating factor for the maintenance of tissue selectivity. A series of raloxifene analogs where this side chain is held in an orientation which is orthogonal to the stilbene plane, similar to the low-energy conformation predicted for raloxifene were constructed. These analogs were prepd. and tested for their activity in a series of in vitro and in vivo biol. assays reflective of the SERM profile. The ability of these analogs to (1) bind the estrogen receptor, (2) antagonize estrogen-stimulated proliferation of MCF-7 cells in vitro, (3) stimulate TGF-.beta.3 gene expression in cell culture, (4) inhibit the uterine effects of ethynyl estradiol in immature rats, and (5) potently reduce serum cholesterol and **protect** against osteopenia in ovariectomized (OVX) rats without estrogen-like stimulation of uterine tissue is detailed. These data demonstrate that LY357489 (I) is among the most potent SERMs described to date with in vivo efficacy on bone and cholesterol metab. in OVX rats at doses as low as 0.01 mg/kg/d.

IT **57-63-6**, 17.alpha.-Ethynyl estradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of conformationally restricted raloxifene analogs and **pharmacol**. as selective estrogen receptor modulators)

L30 ANSWER 10 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:692886 HCAPLUS
DOCUMENT NUMBER: 128:31916
TITLE: Synthesis of 17.alpha.-ruthenocenyl-17.beta.-estradiol and its potential as a radiopharmaceutical agent
AUTHOR(S): Tang, Jie; Top, Siden; Vessieres, Anne; Sellier, Nicole; Vaissermann, Jacqueline; Jaouen, Gerard
CORPORATE SOURCE: Lab. Chimie Organometallique, Ecole Natl. Superieure Chimie Paris, URA CNRS 403, Parix, 75231, Fr.
SOURCE: Applied Organometallic Chemistry (1997), 11(10 & 11), 771-781
CODEN: AOCHEX; ISSN: 0268-2605
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of 17.alpha.-ruthenocenyl-17.beta.-estradiol and results of biochem. tests to det. its suitability as a radiopharmaceutical agent, are

reported. 17.alpha.-Ruthenocyl-17.beta.-estradiol was obtained, in an overall yield of 29%, by addn. of ruthenocenyl-lithium (prepd. by treatment of ruthenocene with t-butyl-lithium) to the ketone function of **protected** estrone, followed by the **deprotection** of the 3-OH function. It was characterized by X-ray crystallog.: space group P 21 (monoclinic), a=9.150(2) .ANG., b=11.806(4) .ANG., c=12.193(3) .ANG., .beta.=94.56(2).degree., V=1313(2) .ANG.3, Z=2. The relative binding affinity (RBA) of this complex for the estradiol-specific receptor was compared with that of estradiol. 17.alpha.-Ruthenocyl-17.beta.-estradiol is still recognized by the estradiol receptor with an RBA of 2%. Unlike its analog, 17.alpha.-propynyl-Co2(CO)5-17.beta.-estradiol, it does not act as an affinity marker for the estradiol receptor. This may be explained by the relative stability of the carbenium ion generated from it, which has a pKR+ value of +0.73. 17.alpha.-Ruthenocyl-17.beta.-estradiol is however of potential interest as a radiopharmaceutical agent since ruthenium has radioactive isotopes emitting .beta.- and .gamma.-radiation useful in nuclear medicine.

IT **101859-59-0 128138-05-6 128138-06-7**
142722-18-7 199458-57-6
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(synthesis of 17.alpha.-ruthenocenyl-17.beta.-estradiol and its potential as **radiopharmaceutical** agent)

IT **199458-53-2P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(synthesis of 17.alpha.-ruthenocenyl-17.beta.-estradiol and its potential as **radiopharmaceutical** agent)

IT **199458-58-7 199458-59-8**
RL: PRP (Properties)
(synthesis of 17.alpha.-ruthenocenyl-17.beta.-estradiol and its potential as **radiopharmaceutical** agent)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 11 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:623043 HCAPLUS
DOCUMENT NUMBER: 127:243636
TITLE: Sequential estrogen/progesterone antagonist combination for hormone replacement therapy
INVENTOR(S): Chwalisz, Kristof
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany; Chwalisz, Kristof
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9733589	A1	19970918	WO 1997-DE580	19970311
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19610635	A1	19970918	DE 1996-19610635	19960311

CA 2248841	AA	19970918	CA 1997-2248841	19970311
AU 9726911	A1	19971001	AU 1997-26911	19970311
EP 889727	A1	19990113	EP 1997-920535	19970311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI				
BR 9708162	A	19990727	BR 1997-8162	19970311
JP 2000506175	T2	20000523	JP 1997-532200	19970311
NO 9804166	A	19980910	NO 1998-4166	19980910
PRIORITY APPLN. INFO.:			DE 1996-19610635	19960311
			WO 1997-DE580	19970311

AB A combination of individual metering units of an estrogen and individual metering units of a competitive progesterone antagonist for the sep. sequential administration thereof, and a pack contg. these units, are provided for hormone replacement therapy. Administration of the progesterone antagonist over a period subsequent to the estrogen administration inhibits the estrogen-induced endometrial proliferation (which may lead to endometrial carcinoma) and decreases the amt. of estrogen-dependent irregular bleeding, but does not interfere with the **protective** effect on estrogen on the bones. The estrogen is typically administered orally, transdermally, or vaginally for 28-112 days, followed by a period of progesterone antagonist administration for 4-30 days.

IT **57-63-6**, Ethynylestradiol **313-06-4**, Estradiol 17-cypionate **979-32-8**, Estradiol 17-valerate **3571-53-7**, Estradiol 17-undecylate **4956-37-0**, Estradiol 17-enanthate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sequential estrogen/progesterone antagonist combination for hormone replacement **therapy**)

L30 ANSWER 12 OF 25 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1997:391697 HCAPLUS
DOCUMENT NUMBER:	127:14340
TITLE:	ATP-dependent transport of aflatoxin B1 and its glutathione conjugates by the product of the multidrug resistance protein (MRP) gene
AUTHOR(S):	Loe, Douglas W.; Stewart, Richard K.; Massey, Thomas E.; Deeley, Roger G.; Cole, Susan P.
CORPORATE SOURCE:	Cancer Research Laboratories, Queen's Univ., Kingston, ON, K7L 3N6, Can.
SOURCE:	Molecular Pharmacology (1997), 51(6), 1034-1041 CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER:	Williams & Wilkins
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Glutathione-S-transferase-catalyzed conjugation of glutathione (GSH) to aflatoxin B1-8,9-epoxide plays an important role in preventing binding of this ultimate carcinogen to target macromols. Once formed, the aflatoxin B1 epoxide-GSH conjugates are actively extruded from the cell by an unidentified ATP-dependent export pump or pumps. Two possible candidates for this GSH conjugate pump are the 190-kDa multidrug resistance protein (MRP) and the 170 kDa P-glycoprotein. Both proteins belong to the ATP-binding cassette superfamily of transmembrane transport proteins and confer resistance to a similar spectrum of natural-product drugs. Using membrane vesicles from MRP-transfected cells, we found that MRP transports GSH conjugates of both the endo-isomers and exo-isomers of aflatoxin B1-8,9-epoxide in an ATP-dependent, osmotically sensitive manner (Vmax = 180 pmol/mg/min, Km = 189 nM). Membrane vesicles from P-glycoprotein-overexpressing cells showed very low levels of transport. MRP-mediated transport was inhibited by an MRP-specific monoclonal antibody and by a variety of GSH derivs. and cholestatic steroid glucuronides. ATP-dependent transport of unmodified aflatoxin B1 by

MRP-enriched membrane vesicles was low but markedly enhanced in the presence of 5 mM GSH, even though GSH conjugates of aflatoxin B1 was not formed by the vesicles. These data demonstrate that MRP is capable of energy-dependent transport of aflatoxin B1 and its GSH conjugates and suggest a potential **protective** role for MRP in mammalian chem. carcinogenesis.

IT **1806-98-0 7219-89-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(ATP-dependent transport of aflatoxin B1 and glutathione conjugates by product of **multidrug** resistance protein (MRP) gene)

L30 ANSWER 13 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:102331 HCAPLUS
DOCUMENT NUMBER: 126:181533
TITLE: Differential effects of hormone-replacement therapy on endogenous nitric oxide (nitrite/nitrate) levels in postmenopausal women substituted with 17.beta.-estradiol valerate and cyproterone acetate or medroxyprogesterone acetate
AUTHOR(S): Imthurn, Bruno; Rosselli, Marinella; Jaeger, Adrian W.; Keller, Paul J.; Dubey, Raghvendra K.
CORPORATE SOURCE: Clinic of Endocrinology, Department of Gynecology and Obstetrics, University Hospital Zurich, Zurich, Switz.
SOURCE: Journal of Clinical Endocrinology and Metabolism (1997), 82(2), 388-394
CODEN: JCEMAZ; ISSN: 0021-972X
PUBLISHER: Endocrine Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Increased incidence of cardiovascular disease in postmenopausal women (PMW) is accompanied by ovarian dysfunction; hormone replacement therapy (HRT) can have **cardioprotective** effects. Because hypertension and atherosclerosis are assocd. with impaired release of endothelium-derived nitric oxide (NO) and increased levels of low-d. lipoproteins (LDL), the authors investigated whether HRT augments NO release, and whether these increases are accompanied by a decrease in LDL levels in PMW. The authors detd. serum nitrite/nitrate (NO2-/NO3-) and LDL levels at baseline (before initiation of HRT) and during the 6th and 12th months of the study. The PMW received continuous oral administration of estradiol valerate (Progynova, 2 mg daily) for 21 days supplemented with either oral cyproterone acetate (CPA; 1 mg) or medroxyprogesterone acetate (MPA; 5 mg) on days 12-21 of each treatment cycle. Blood samples in the PMW receiving HRT were collected at times while the subjects were taking estradiol valerate alone and estradiol valerate plus CPA or MPA. Compared with the samples collected at baseline, serum NO2-/NO3- levels increased significantly from 20.1 .mu.M at baseline to 30 .mu.M in samples collected after 12 mo of HRT while the PMW were not taking progestins (CPA or MPA), and to 25.4 .mu.M when all the samples, regardless of the treatment with CPA or MPA, were included in the anal. Moreover, >30% increase in serum NO2-/NO3- levels were obsd. only in 13 (responders) out of 26 PMW substituted with estradiol valerate, suggesting that estradiol may improve endogenous NO synthesis in a differential fashion. Compared with baseline, no significant increases in serum NO2-/NO3- were obsd. in samples collected while the estradiol-treated responders were taking either CPA or MPA. In contrast to NO2-/NO3-, serum LDL levels were significantly reduced in samples collected after 12 mo of HRT (vs. baseline). Furthermore, levels of NO2-/NO3 showed a significant neg. correlation with the levels of LDL (R2 = 0.17) in the responders but not in nonresponders. These results indicate that oral administration of estradiol valerate in PMW for HRT increases circulating NO levels, an effect that may contribute to the **cardioprotective** effects of HRT in PMW. In addn., the authors' data suggests but does not prove that

concomitant administration of a progestin may attenuate the beneficial effects of estrogen replacement therapy with regard to NO release. Finally the authors' data provides evidence for the existence of responders and nonresponders to postmenopausal estrogen treatment with respect to improvement of endogenous NO levels, suggesting that a significant no., but not all, of the hormonally substituted PMW profit fully from the beneficial properties of a HRT.

IT **979-32-8**, Progynova
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(differential effects of hormone-replacement **therapy** on endogenous nitric oxide levels in postmenopausal women substituted with estradiol and cyproterone or medroxyprogesterone acetate)

L30 ANSWER 14 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:709429 HCAPLUS
DOCUMENT NUMBER: 125:317913
TITLE: The comparative effect on bone density, endometrium, and lipids of continuous hormones as replacement therapy (CHART study). A randomized controlled trial
AUTHOR(S): Speroff, Leon; Rowan, Jean; Symons, James; Genant, Harry; Wilborn, Walter
CORPORATE SOURCE: Department Obstetrics and Gynecology, Oregon Health Sciences University, Portland, USA
SOURCE: JAMA, the Journal of the American Medical Association (1996), 276(17), 1397-1403
CODEN: JAMAAP; ISSN: 0098-7484
PUBLISHER: American Medical Association
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To compare the effect of continuous norethindrone acetate (NA)-ethinyl estradiol (EE2) combinations with matching unopposed EE2 or placebo. Patients included asymptomatic or mildly symptomatic women aged 40 yr or older who had undergone the onset of spontaneous menopause within the last 5 yr and who had an intact uterus. Patients were equally randomized to placebo or 1 of 8 treatment groups: 0.2 mg of NA and 1 .mu.g of EE2; 0.5 mg of NA and 2.5 .mu.g of EE2; 1 mg of NA and 5 .mu.g of EE2; 1 mg of NA and 10 .mu.g of EE2; 1 .mu.g of EE2; 2.5 .mu.g of EE2; 5 .mu.g of EE2; or 10 .mu.g of EE2. Primary outcome measures included bone mineral d. (BMD) measured by quant. computed tomog., serum lipids, and endometrial effects as assessed by rate of hyperplasia and proliferative status. Twelve hundred sixty-five patients entered the study. Bone mineral d. increased significantly from baseline in the 1 mg NA-5 .mu.g EE2 and the 1 mg NA-10 .mu.g EE2 treatment groups at each annual assessment. Among the unopposed EE2 groups, only the 10-.mu.g group had increased BMD above baseline, but also was accompanied by an unacceptably high rate of endometrial hyperplasia. The NA-EE2 treatment groups had a significant linear dose-response trend for increasing BMD. Increased endometrial proliferation and hyperplasia occurred with increasing unopposed estrogen doses. The combination of NA and EE2 effectively **protected** the endometrium against hyperplasia. The percentage of change in the ratio of high-d. lipoprotein cholesterol to low-d. lipoprotein cholesterol was pos. for all treatment groups. The increase in triglyceride levels assocd. with EE2 was attenuated with NA-EE2 treatment. Daily treatment with NA-EE2 was well tolerated and **protected** the endometrium from EE2-induced proliferation and hyperplasia. The NA-EE2 treatments produced a dose-related significant increase in BMD that was not present with unopposed EE2 treatment. The overall effect of NA-EE2 treatments on lipid measures was favorable.

IT **57-63-6**, Ethynylestradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparative effect on bone d., endometrium, and lipids of continuous

hormones as replacement **therapy** in humans)

L30 ANSWER 15 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:435753 HCAPLUS
DOCUMENT NUMBER: 125:76843
TITLE: Serotonin metabolite excretion after postmenopausal estradiol therapy
AUTHOR(S): Lippert, Theodor H.; Filshie, Marcus; Mueck, Alfred O.; Seeger, Harald; Zwirner, Manfred
CORPORATE SOURCE: Department Obstetrics and Gynecology, Tubingen, 72 076, Germany
SOURCE: Maturitas (1996), 24(1,2), 37-41
CODEN: MATUDK; ISSN: 0378-5122
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Serotonin, known for its beneficial action on mood and well-being, is also involved in cardiovascular functions. Thus the current work was undertaken to study the effect of hormone replacement therapy on serotonin turnover in postmenopausal women. Eighteen women received estradiol transdermally and 17 women estradiol valerate orally for 4 wk. The serotonin metabolite 5-hydroxyindole acetic acid (5-HIAA) was detd. in the urine before, and after 2 and 4 wk' estradiol treatment. With both administration routes estradiol produced a significant increase in urinary 5-HIAA excretion, greatest with transdermal estradiol after 28 days of treatment. The enhancement of serotonin turnover may contribute not only to an improvement of mood and well-being but also to a **cardioprotective** effect of estradiol obsd. after hormone substitution in postmenopausal women.
IT **979-32-8**, Estradiol valerate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(serotonin metabolite excretion after postmenopausal estradiol **therapy**, in humans)

L30 ANSWER 16 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:946993 HCAPLUS
DOCUMENT NUMBER: 123:350257
TITLE: Pharmaceutical compositions containing a steroidal active agent and a fatty acid ester of ascorbic acid as antioxidant
INVENTOR(S): Hilmann, Juergen
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4412464	A1	19951026	DE 1994-4412464	19940408

PRIORITY APPLN. INFO.: DE 1994-4412464 19940408
AB Esters of C10-20 fatty acids with ascorbic acid **protect** steroids from oxidn. at the C-6 position. Thus, tablets contg. ethynylestradiol were stabilized by addn. of 1-2% ascorbic acid palmitate.
IT **57-63-6**, Ethynylestradiol **979-32-8**, Estradiol valerate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**pharmaceutical** compns. contg. steroidal active agent and fatty acid ester of ascorbic acid as antioxidant)

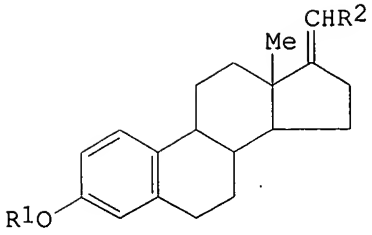
L30 ANSWER 17 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:687045 HCAPLUS
DOCUMENT NUMBER: 115:287045
TITLE: Oral bioavailability of 17.beta.-estradiol and various ester prodrugs in the rat
AUTHOR(S): Lokind, Kenneth B.; Lorenzen, Finn Hjort; Bundgaard, Hans
CORPORATE SOURCE: Dep. Pharm., Novo Nordisk A/S, Bagsvaeerd, Den.
SOURCE: International Journal of Pharmaceutics (1991), 76(1-2), 177-82
CODEN: IJPHDE; ISSN: 0378-5173
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The oral bioavailability of 17.beta.-estradiol is only about 10% in humans due to extensive first-pass metab. The feasibility of depressing this metab. and hence improving the systemic bioavailability by the prodrug approach was examd. using a rat model. The prodrugs studied included the 17-acetate, 17-valerate, 17-cypionate, 3-benzoate, 3-acetylsalicylate and 3-anthranilate esters of 17.beta.-estradiol. Following oral administration to rats the systemic bioavailability of 17.beta.-estradiol was 4.3% whereas the bioavailability obsd. after administration of the esters ranged from 1.0 to 7.6%. The esters are unable to **protect** the parent drug against first-pass metab. as assessed in the rat. The poor bioavailability obsd. with the 3-acetylsalicylate and 3-anthranilate esters contrasts greatly with previously reported findings with these ester prodrugs in dogs.
IT **313-06-4**, Estradiol 17.beta.-cypionate **979-32-8**, Estradiol 17.beta.-valerate **1743-60-8**
RL: PROC (Process)
(oral bioavailability of, as estradiol **prodrug**)

L30 ANSWER 18 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:614810 HCAPLUS
DOCUMENT NUMBER: 111:214810
TITLE: Preparation, testing, and formulation of 17-(halomethylene)-1,3,5(10)-estratrien-3-ols as drugs
INVENTOR(S): Jungblut, Peter; Wiechert, Rudolf; Bohlmann, Rolf
PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 5 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3741800	A1	19890615	DE 1987-3741800	19871207
EP 320438	A1	19890614	EP 1988-730274	19881205
EP 320438	B1	19920923		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 80893	E	19921015	AT 1988-730274	19881205
ES 2045176	T3	19940116	ES 1988-730274	19881205
JP 01193295	A2	19890803	JP 1988-307067	19881206
JP 2636913	B2	19970806		
CA 1324374	A1	19931116	CA 1988-585131	19881206
AU 8826652	A1	19890608	AU 1988-26652	19881207
AU 617140	B2	19911121		
US 5124321	A	19920623	US 1988-280912	19881207

PRIORITY APPLN. INFO.: DE 1987-3741800 19871207
EP 1988-730274 19881205

OTHER SOURCE(S): MARPAT 111:214810
GI



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AB The title compds. (I; R1 = H, Me, acyl; R2 = halo), useful as contraceptive components and for treating hormone-dependent tumors and estradiol deficit, were prepd. FCH2P+Ph3 BF4- in dioxane was stirred 0.5 h with KOCMe3 at 20.degree.. 1,3,5(10)Estrratrien-3-ol-17-one in dioxane was added and the mixt. was stirred 30 min to give (E,Z)-17-fluoromethylene-1,3,5(10)estratrien-3-ol (II). In rats II had 1/40th of the uterotropic activity of estradiol. I inhibited growth of mammary tumors in rats and in therapeutically castrated women I alleviated bone pain and hot flashes.

IT **123651-64-9P 123651-69-4P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as **drug**)

L30 ANSWER 19 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:529463 HCAPLUS
DOCUMENT NUMBER: 109:129463
TITLE: New 11-(alkynylphenyl)-substituted 19-nor and 19-nor-D-homo steroids, their formation and pharmacological activity, and processes for their preparation
INVENTOR(S): Teutsch, Jean Georges; Klich, Michel; Philibert, Daniel
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 88 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 245170	A1	19871111	EP 1987-401018	19870504
EP 245170	B1	19891129		
R: CH, DE, GB, IT, LI, NL, SE				
FR 2598421	A1	19871113	FR 1986-6517	19860506
FR 2598421	B1	19880819		
US 4912097	A	19900327	US 1987-44958	19870430
HU 44793	A2	19880428	HU 1987-2007	19870505
HU 196224	B	19881028		
JP 62294694	A2	19871222	JP 1987-109059	19870506

PRIORITY APPLN. INFO.: FR 1986-6517 19860506
OTHER SOURCE(S): CASREACT 109:129463
GI For diagram(s), see printed CA Issue.
AB Title steroids I [R1 = C2-8 alkynyl (un)substituted by OH, halo, trialkylsilyl, alkoxy, alkylthio, dialkylamino, or oxo; R2 = C1-3 alkyl; A/B-rings = Q1-Q5; D-ring = Q6, Q7; R3, R4 = H, C1-4 alkyl; R5 = H, OH, acycloxy, (un)substituted C1-6 alkoxy; R6 = H, C1-8 alkyl, C7-15 aralkyl; R7, R8 = H, OH, etc.; R7R8 = lactones and related groups; YZ = CH2CH2,

CH:CH, 1,2-cyclopropanediyl, CHR9CH2, CH2CHR10; R9, R10 = C1-4 alkyl] are prepd. for use as progestogens, antiprogestogens, and/or antiglucocorticoids. 3,3-Ethylenedioxy-5,10-epoxy-estr-9(11)-en-17-one was treated with 4-(Me3SiC:C)C6H4MgBr and CuCl in THF, and the product treated with CH2:CHCH2MgBr and **deprotected** and dehydrated (NH4OH in aq. MeOH, then aq. HCl) to give (ethylnylphenyl)allylhydroxyestradienone II. At 10-6M in vitro, II gave 99% reversal of the dexamethasone-induced redn. of uridine uptake by rat thymocytes (5 .times. 10-8M dexamethasone). Tablets were prepd. from 50 mg of the 17.alpha.-(chloroethynyl) analog of II, and 120 mg of a mixt. of talc, starch, and Mg stearate.

IT **116421-71-7P 116421-72-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as **drug**)

L30 ANSWER 20 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:6287 HCAPLUS
DOCUMENT NUMBER: 108:6287
TITLE: Amino-substituted steroids having a variety of pharmacological activities, and processes for their preparation
INVENTOR(S): McCall, John M.; Jacobsen, E. Jon; Van Doornik, Frederick J.; Palmer, John R.; Karnes, Harold A.
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8701706	A2	19870326	WO 1986-US1797	19860828
WO 8701706	A3	19870716		
W: AU, DK, FI, JP, KR, NO, SU, US, US, US, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
IL 79702	A1	19920216	IL 1986-79702	19860812
IL 98007	A1	19920216	IL 1986-98007	19860812
ZA 8606097	A	19880330	ZA 1986-6097	19860813
CA 1308707	A1	19921013	CA 1986-516177	19860818
AU 8663356	A1	19870407	AU 1986-63356	19860828
AU 593284	B2	19900208		
EP 238545	A1	19870930	EP 1986-905605	19860828
EP 238545	B1	19951115		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 63500868	T2	19880331	JP 1986-504810	19860828
JP 05035158	B4	19930525		
AT 130307	E	19951215	AT 1986-905605	19860828
CN 86106226	A	19870318	CN 1986-106226	19860912
CN 1030319	B	19951122		
DK 8702375	A	19870511	DK 1987-2375	19870511
NO 8701930	A	19870511	NO 1987-1930	19870511
NO 176762	B	19950213		
NO 176762	C	19950531		
FI 8702107	A	19870512	FI 1987-2107	19870512
FI 94417	B	19950531		
FI 94417	C	19950911		
US 5099019	A	19920324	US 1988-229675	19880808
AU 8940806	A1	19891207	AU 1989-40806	19890825
AU 614661	B2	19910905		
AU 8940807	A1	19891207	AU 1989-40807	19890825

AU 614418	B2	19910829		
US 5175281	A	19921229	US 1991-749830	19910826
US 5322943	A	19940621	US 1991-749829	19910826
JP 05112597	A2	19930507	JP 1992-8428	19920121
US 35053	E	19951010	US 1992-959310	19921009
US 5268477	A	19931207	US 1992-977768	19921119
US 5380839	A	19950110	US 1992-983082	19921201
US 5380840	A	19950110	US 1992-983084	19921201
US 5380841	A	19950110	US 1992-984299	19921201
US 5382661	A	19950117	US 1992-984298	19921201
US 5506354	A	19960409	US 1992-984302	19921201

PRIORITY APPLN. INFO.:

US 1985-775204	19850912
US 1985-811058	19851219
US 1986-877287	19860623
US 1986-888231	19860729
IL 1986-79702	19860812
WO 1986-US1797	19860828
US 1987-121822	19870511
US 1988-227812	19880803
US 1988-229675	19880808
US 1991-749829	19910826
US 1991-749830	19910826

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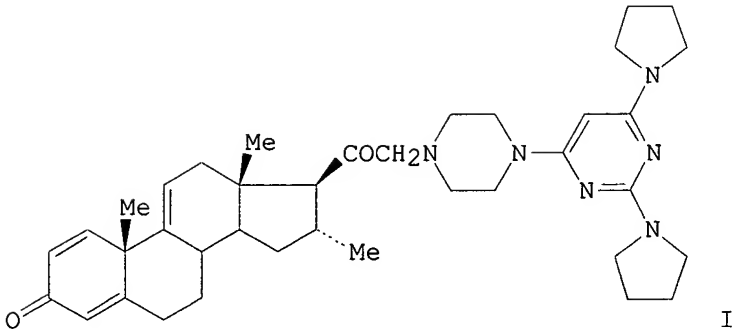


I

AB Numerous pregnane derivs. with amino-substituted sidechains were prepd. for use as various types of drugs. Aminolysis of 21-iodo-16.alpha.-methylpregna-1,4,9(11)-triene-3,20-dione with 4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)piperazine in MeCN contg. K2CO3 at 60.degree. gave [[bis(pyrrolidino)pyrimidinyl]piperazinyl]pregnane deriv. I, which was converted to I.2MeSO3H (II). In the interleukin-1-induced T-cell proliferation assay, II gave 62% inhibition at 10-6 M, thereby demonstrating antiarthritic activity.

IT **111669-04-6P 111669-05-7P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as **drug**)

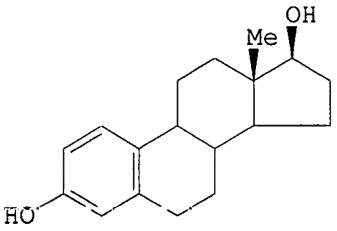
L30 ANSWER 21 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:123370 HCAPLUS
DOCUMENT NUMBER: 104:123370
TITLE: Increased mRNA for low density lipoprotein receptor in livers of rabbits treated with 17.alpha.-ethynylestradiol
AUTHOR(S): Ma, Patrick T. S.; Yamamoto, Tokuo; Goldstein, Joseph L.; Brown, Michael S.
CORPORATE SOURCE: Health Sci. Cent., Southwest. Med. Sch., Univ. Texas, Dallas, TX, 75235, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1986), 83(3), 792-6
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English
AB **Pharmacol**. doses of 17.alpha.-ethynylestradiol [**57-63-6**] increased the no. of low d. lipoprotein (LDL) receptors in livers of male and female rabbits and the increase in receptor no. is correlated with a 6-8-fold increase in the levels of receptor mRNA. Receptor protein was measured by ligand blotting, and mRNA levels were measured by a quant. soln. hybridization/S1 nuclease **protection** assay using uniformly 32P-labeled single-strand cDNA probes. Thus **pharmacol**. induction of the mRNA for the LDL receptor in liver can lead to increased LDL receptor levels and a fall in plasma cholesterol [57-88-5] in exptl. animals.
IT **57-63-6**
RL: BIOL (Biological study)
(low-d. lipoprotein receptor-specifying mRNA of liver increase by)

L30 ANSWER 22 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1982:598 HCAPLUS
DOCUMENT NUMBER: 96:598
TITLE: Effect of inhibition of platelet function with carbenicillin or aspirin on experimental canine sudden death
AUTHOR(S): Johnson, Gerhard J.; Heckel, Richard; Leis, Linda A.; Franciosa, Joseph
CORPORATE SOURCE: Hematol. Sect., VA Med. Cent., Minneapolis, MN, 55417, USA
SOURCE: Journal of Laboratory and Clinical Medicine (1981), 98(5), 660-72
CODEN: JLCMAK; ISSN: 0022-2143
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Coronary artery embolization resulted in acute myocardial ischemia that was followed by sudden death (death within 15 min of embolization) in 51% of anesthetized control dogs. Pretreatment with carbenicillin [4697-36-3], which markedly inhibited platelet aggregation, or estradiol cypionate [**313-06-4**], which induced severe thrombocytopenia, significantly reduced the incidence of sudden death to 9% and zero, resp. Pretreatment with aspirin [50-78-2], which uniformly inhibited platelet aggregation, was assocd. with a reduced incidence of sudden death (25%), but the difference between aspirin-treated and control animals lacked statistical significance. **Drug** treatment did not prevent myocardial infarction, and the sizes of myocardial infarcts obsd. in animals that survived 30 days were not different from those of control animals. Sudden death was preceded by a significantly greater fall in mean arterial pressure than that obsd. in survivors, but the frequency of ventricular ectopic beats did not differ in survivors and nonsurvivors. Apparently, platelets play an important role in exptl. sudden death which follows acute coronary embolization and inhibition of platelet function **protects** against exptl. sudden death by a mechanism that prevents severe hypotension but is not antiarrhythmic. **Drug**-induced platelet dysfunction and thrombocytopenia may **protect** against exptl. sudden death by preventing intravascular platelet aggregation and embolization.
IT **313-06-4**
RL: BIOL (Biological study)
(cardiac sudden death prevention by, thrombocytopenia induction in)

L30 ANSWER 23 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:25592 HCAPLUS
DOCUMENT NUMBER: 94:25592

TITLE: Postcoital contraception with an injectable estrogen preparation (Org 369-2)
AUTHOR(S): Schindler, A. E.; Ladanyi, S.; Goeser, R.; Keller, E.
CORPORATE SOURCE: Dep. Obstet. Gynaecol., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.
SOURCE: Contraception (1980), 22(2), 165-74
CODEN: CCPTAY; ISSN: 0010-7824
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB In 100 women age 15 to 45, postcoital contraception was attempted with a morning-after injection of Org 369-2 [**62322-24-1**], (consisting of 12.5 mg estradiol benzoate and 10 mg estradiol phenylpropionate). Plasma 17.beta.-estradiol (I) [50-28-2], progesterone [57-83-0], LH [9002-67-9], FSH [9002-68-0] and prolactin [9002-62-4] were measured by specific radioimmunoassays. In 97% of the cases the injection was given within 48 h after **unprotected** coitus. The **medication** induced minimal cycle and bleeding pattern changes. The rate of side effects was low. The incidence of pregnancies due to **medication** failure was 3%. The plasma hormone patterns before and under **therapy** are given and **drug**-induced changes discussed.

IT **62322-24-1**
RL: BIOL (Biological study)
(as postcoital contraceptive)

L30 ANSWER 24 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1975:38656 HCAPLUS
DOCUMENT NUMBER: 82:38656
TITLE: Use of a rabbit extracorporeal shunt in the assay of antithrombotic and thrombotic drugs
AUTHOR(S): Rosenberg, Franklin J.; Phillips, Patricia G.; Druzba, Patricia R.
CORPORATE SOURCE: Sterling-Winthrop Res. Inst., Rensselaer, NY, USA
SOURCE: Platelets Thromb., Proc. Symp. (1974), Meeting Date 1972, 223-34. Editor(s): Sherry, Sol. Univ. Park Press: Baltimore, Md.
CODEN: 29ELAC
DOCUMENT TYPE: Conference
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Tests on rabbits with carotid-jugular extracorporeal shunts showed that acetylsalicylic acid (I) [50-78-2] and hydroxychloroquine [118-42-3] each inhibited thrombus formation without affecting blood pressure or flow. Both **drugs** reduced platelet consumption, and I reduced it in relation to the redn. in thrombus wt. The estrogens ethynylestradiol [**57-63-6**] and mestranol [72-33-3] increased thrombus wts. and decreased bleeding in a dose-dependent fashion. Contraceptive **drug** combinations contg. these estrogens had less effects on thrombus wts. than did the pure estrogens. This **protective** effect could not be related to an antithrombotic effect of the progestins.

IT **57-63-6**
RL: BIOL (Biological study)
(thrombus formation response to)

L30 ANSWER 25 OF 25 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1971:544001 HCAPLUS
DOCUMENT NUMBER: 75:144001
TITLE: Therapeutic compositions consisting of a progestogan, and estrogen, and a vascular and hepatic **protector**, for treating hormonal dysfunctions
INVENTOR(S): Bouchara, Emile
SOURCE: Fr. M., 2 pp.
CODEN: FMXXAJ
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 6955		19690630	FR	19670724

AB A medical compn. which relieved hormonal disorders, e.g. ovulation disorders, contained a progestatorial hormone such as 17.alpha.-ethynyl-19-nortestosterone or [17.alpha.-ethynyl-17.beta.-hydroxy-5(10)-estren-3-one], a synthetic estrogenic hormone such as ethynylestradiol, a vascular **protector** such as rutoside or tris-O-(2-hydroxyethyl)-rutin, and an hepatic guard, such as [tris(p-methoxyphenylthio)-propene] or bromo(hydroxy)naphthoic acid. This compn. was administered orally in the form of a lozenge or gel.
IT **57-63-6**
RL: BIOL (Biological study)
(**pharmaceutical**)

=> select hit rn 130 1-25
E7 THROUGH E30 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 19:49:34 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9
DICTIONARY FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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1 979-32-8/BI

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L31         24 (979-32-8/BI OR 57-63-6/BI OR 313-06-4/BI OR 1806-98-0/BI OR
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                7/BI OR 116421-72-8/BI OR 123651-64-9/BI OR 123651-69-4/BI OR
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                199458-59-8/BI OR 3571-53-7/BI OR 4956-37-0/BI OR 62322-24-1/BI
                OR 71138-35-7/BI OR 7219-89-8/BI)

=>
=> d ide can l31 1-24

L31  ANSWER 1 OF 24  REGISTRY  COPYRIGHT 2003 ACS
RN   199458-59-8  REGISTRY
CN   Estra-1,3,5(10)trien-17-ylium, 3-hydroxy-17-ruthenocenyl- (9CI)  (CA INDEX
     NAME)
MF   C28 H31 O Ru
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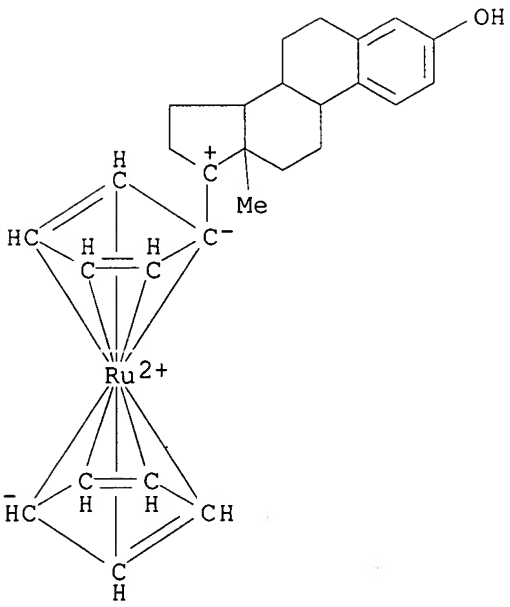
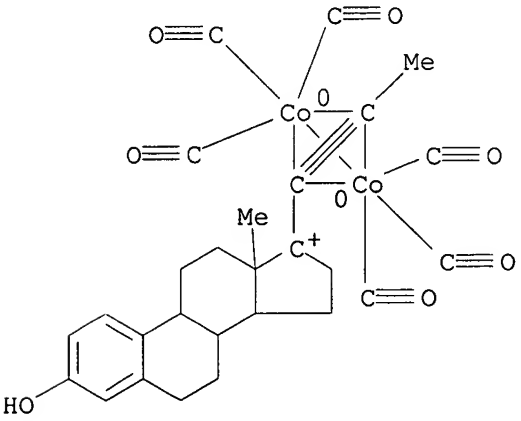
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:31916

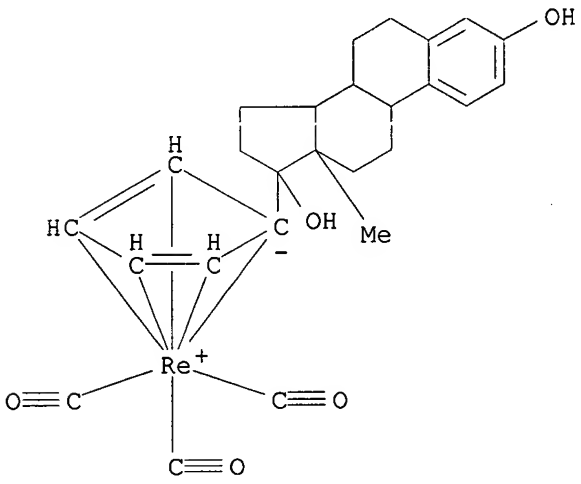
L31 ANSWER 2 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **199458-58-7** REGISTRY
CN Cobalt(1+), hexacarbonyl[.mu.-[3-hydroxy-17-[(1,2-.eta.:1,2-.eta.)-1-propynyl]estra-1,3,5(10)trien-17-ylium]]di-, (Co-Co) (9CI) (CA INDEX NAME)
MF C27 H25 Co2 O7
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:31916

L31 ANSWER 3 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **199458-57-6** REGISTRY
CN Rhenium, tricarbonyl[(1,2,3,4,5-.eta.)-1-[(17.beta.)-3,17-dihydroxyestra-1,3,5(10)trien-17-yl]-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)
MF C26 H27 O5 Re
CI CCS
SR CA
LC STN Files: CA, CAPLUS

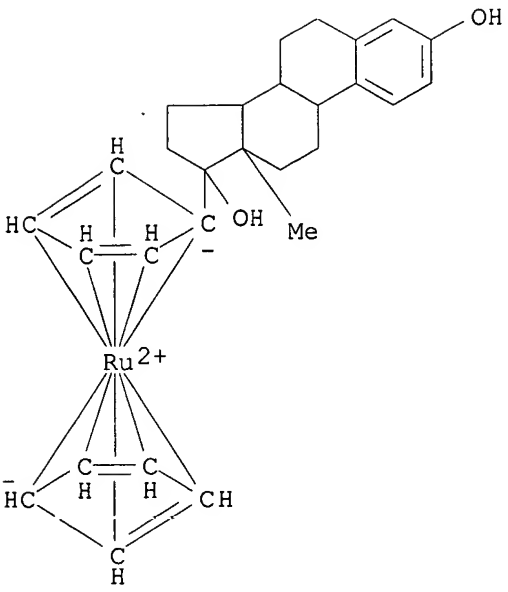


2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 130:196799

REFERENCE 2: 128:31916

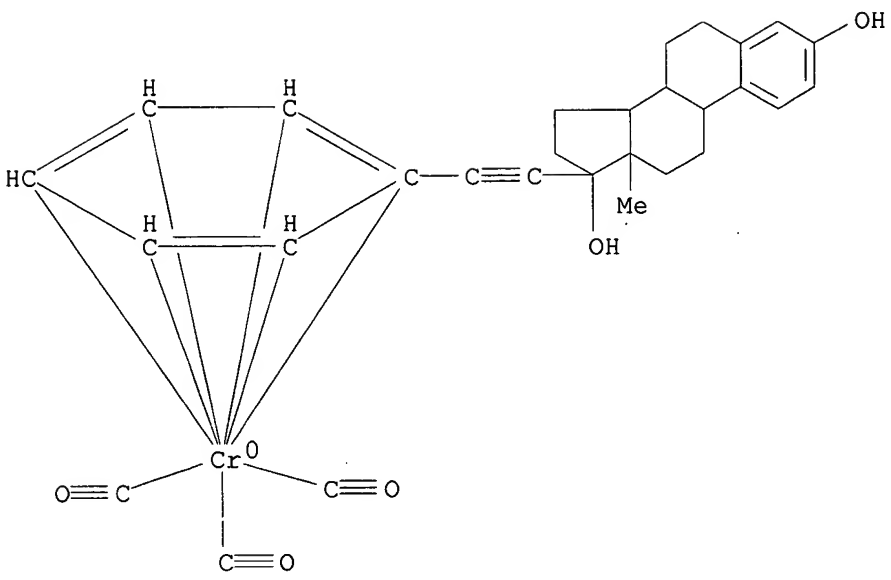
L31 ANSWER 4 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **199458-53-2** REGISTRY
CN Ruthenocene, [(17.beta.)-3,17-dihydroxyestra-1,3,5(10)trien-17-yl]- (9CI) (CA INDEX NAME)
MF C28 H32 O2 Ru
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:31916

L31 ANSWER 5 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **142722-18-7** REGISTRY
CN Chromium, tricarbonyl[(17.alpha.)-21-(.eta.6-phenyl)-19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregnane, chromium deriv.
MF C29 H28 Cr O5
CI CCS
SR CA
LC STN Files: CA, CAPLUS



4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

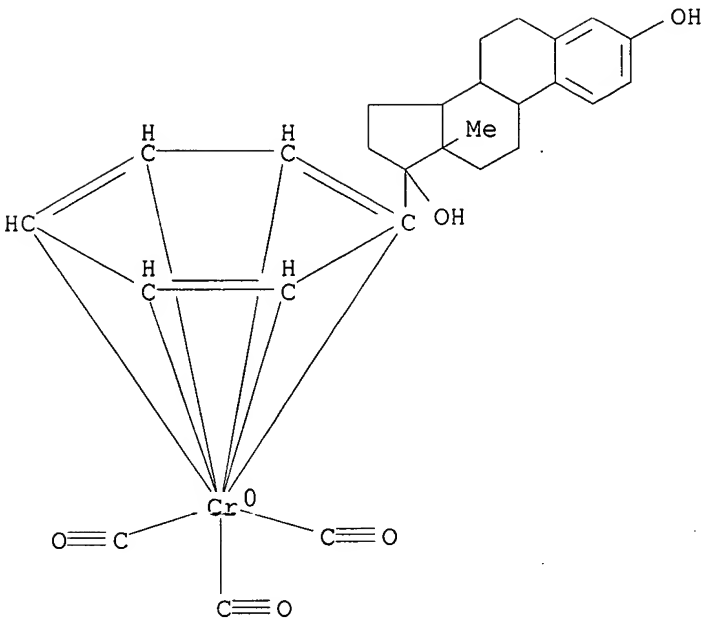
REFERENCE 1: 128:31916

REFERENCE 2: 123:257119

REFERENCE 3: 122:306655

REFERENCE 4: 117:104388

L31 ANSWER 6 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **128138-06-7** REGISTRY
CN Chromium, tricarbonyl[(17.beta.)-17-(.eta.6-phenyl)estra-1,3,5(10)-triene-3,17-diol]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,17-diol, 17-phenyl-, chromium complex, (17.beta.)-
CN Estrane, chromium deriv.
MF C27 H28 Cr O5
CI CCS
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:31916

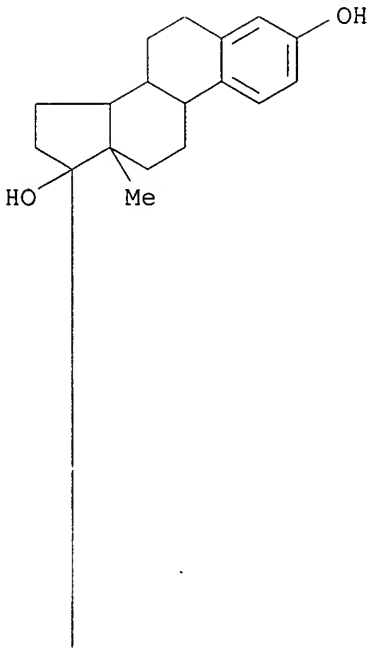
REFERENCE 2: 123:257119

REFERENCE 3: 117:104388

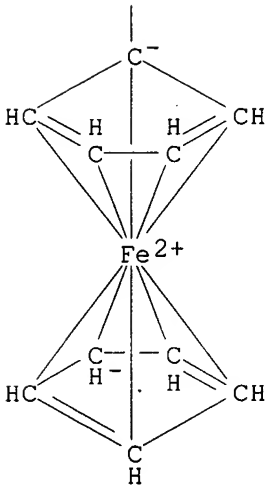
REFERENCE 4: 113:35456

L31 ANSWER 7 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **128138-05-6** REGISTRY
CN Ferrocene, [(17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-17-yl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estrane, ferrocene deriv.
OTHER NAMES:
CN 17.alpha.-Ferrocenylestradiol
MF C28 H32 Fe O2
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

PAGE 1-A



PAGE 2-A



6 REFERENCES IN FILE CA (1962 TO DATE)
6 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:31916

REFERENCE 2: 122:265748

REFERENCE 3: 120:290263

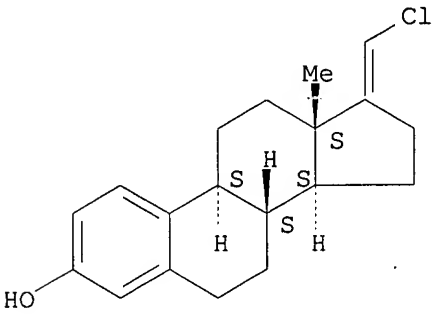
REFERENCE 4: 117:104388

REFERENCE 5: 113:212419

REFERENCE 6: 113:35456

L31 ANSWER 8 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **123651-69-4** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(chloromethylene)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17-(Chloromethylene)-1,3,5(10)-estratrien-3-ol
FS STEREOSEARCH
MF C19 H23 Cl O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



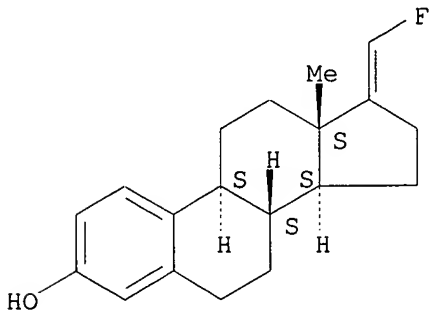
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:214810

L31 ANSWER 9 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **123651-64-9** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(fluoromethylene)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17-(Fluoromethylene)-1,3,5(10)-estratrien-3-ol
FS STEREOSEARCH
MF C19 H23 F O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



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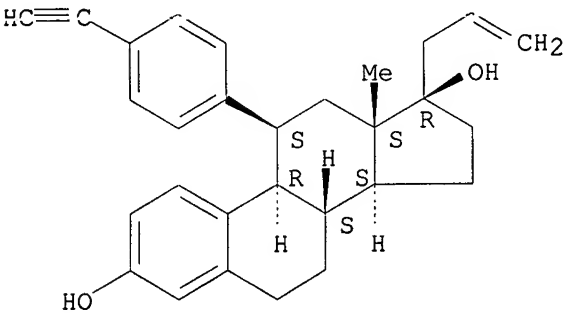
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:214810

L31 ANSWER 10 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **116421-72-8** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-(4-ethynylphenyl)-17-(2-propenyl)-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H32 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



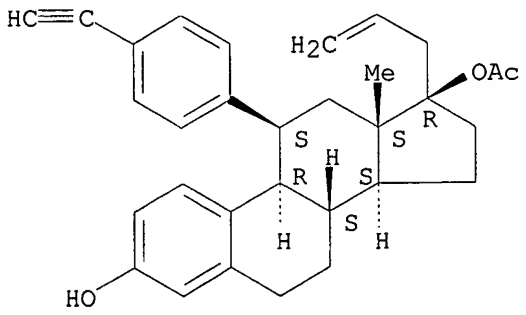
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 109:129463

L31 ANSWER 11 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **116421-71-7** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 11-(4-ethynylphenyl)-17-(2-propenyl)-, 17-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H34 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

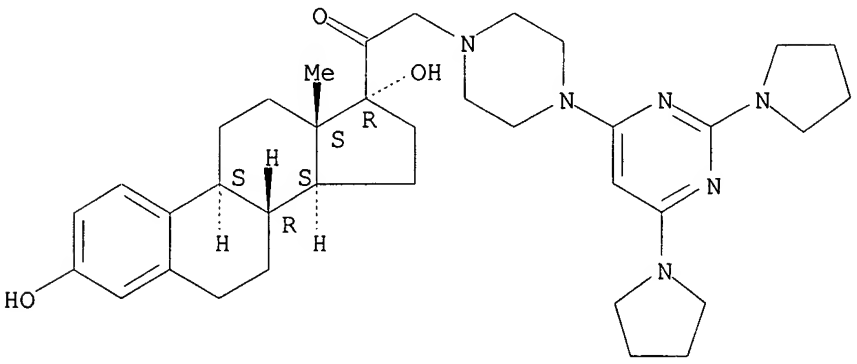
REFERENCE 1: 109:129463

L31 ANSWER 12 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **111669-05-7** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3,17-dihydroxy-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregna-1,3,5(10)-trien-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3,17-dihydroxy-, (E)-2-butenedioate (1:1) (salt)
FS STEREOSEARCH
MF C36 H50 N6 O3 . C4 H4 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

CRN 111669-04-6
CMF C36 H50 N6 O3

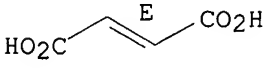
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



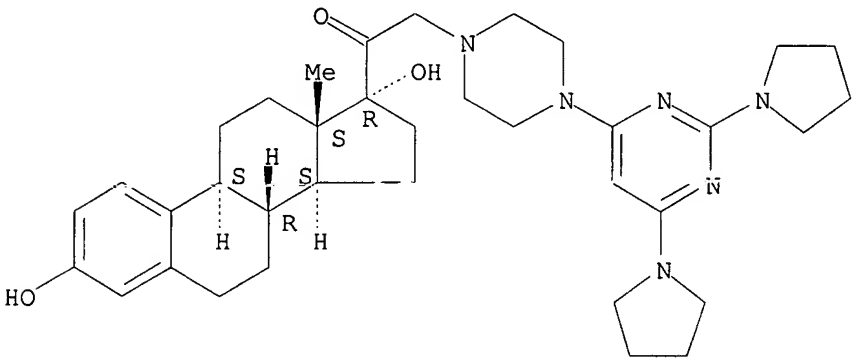
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 109:231361

REFERENCE 2: 108:6287

L31 ANSWER 13 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **111669-04-6** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3,17-dihydroxy- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H50 N6 O3
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 109:231361

REFERENCE 2: 108:6287

L31 ANSWER 14 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **101859-59-0** REGISTRY
CN Cobalt, hexacarbonyl[.mu.-[(17.beta.)-17-[(1,2-.eta.:1,2-.eta.)-1-propynyl]estra-1,3,5(10)-triene-3,17-diol]]di-, (Co-Co) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,17-diol, 17-(1-propynyl)-, cobalt complex, (17.beta.)-
CN Estrane, cobalt deriv.
DR 109282-00-0
MF C27 H26 Co2 O8
CI CCS
SR CA
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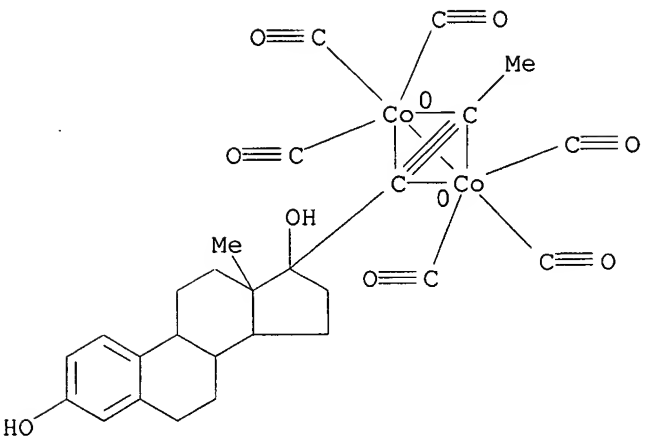


9 REFERENCES IN FILE CA (1962 TO DATE)
9 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:322021

REFERENCE 2: 128:31916

REFERENCE 3: 117:40642

REFERENCE 4: 115:178518

REFERENCE 5: 114:131655

REFERENCE 6: 112:132610

REFERENCE 7: 109:142683

REFERENCE 8: 105:111328

REFERENCE 9: 105:6672

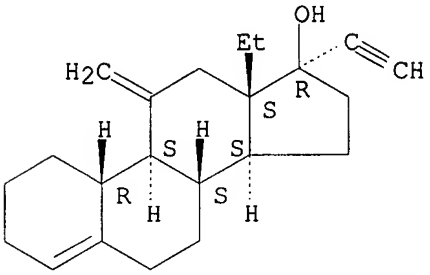
L31 ANSWER 15 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **71138-35-7** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)-, mixt. with (17.alpha.)-13-ethyl-11-methylene-18,19-dinorpregn-4-en-20-yn-17-ol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 18,19-Dinorpregn-4-en-20-yn-17-ol, 13-ethyl-11-methylene-, (17.alpha.)-, mixt. contg. (9CI)
OTHER NAMES:
CN CTR 24
CN Cycleane
CN Cyclessa
CN Desogen
CN Desogen (contraceptive)
CN Desogestrel-ethinylestradiol mixt.
CN Desogestrel-ethylnylestradiol mixture
CN Desogestrel-ethynylestradiol mixt.
CN Desolett
CN Ethinylestradiol-desogestrel mixt.
CN Gracial
CN Laurina
CN Lovelle
CN Marvelon

CN Mercilon
CN Mircette
CN Novelon
CN Org 5187
CN Ortho Cept
CN Ovidol
CN Oviol
CN Practil 2
CN Relivon
FS STEREOSEARCH
MF C22 H30 O . C20 H24 O2
CI MXS
LC STN Files: ADISNEWS, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CBNB, CIN, DIOGENES, DRUGNL, DRUGPAT, DRUGUPDATES, EMBASE, MEDLINE, MRCK*, PHAR, PHARMASEARCH, PROMT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

CM 1

CRN 54024-22-5
CMF C22 H30 O

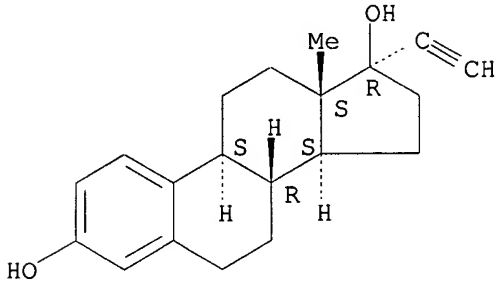
Absolute stereochemistry. Rotation (+).



CM 2

CRN 57-63-6
CMF C20 H24 O2

Absolute stereochemistry.



229 REFERENCES IN FILE CA (1962 TO DATE)
229 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:198882

REFERENCE 2: 138:198881

REFERENCE 3: 138:198877

REFERENCE 4: 138:117744

REFERENCE 5: 138:101085

REFERENCE 6: 138:19652

REFERENCE 7: 137:380158

REFERENCE 8: 137:346420

REFERENCE 9: 137:135235

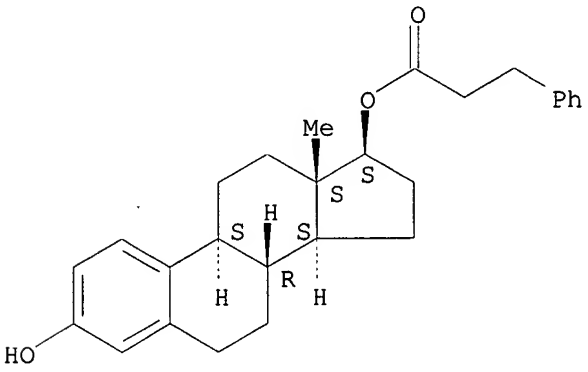
REFERENCE 10: 137:104002

L31 ANSWER 16 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **62322-24-1** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-benzenepropanoate, mixt. with (17.beta.)-17-hydroxyestra-1,3,5(10)-trien-3-yl benzoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 3-benzoate, mixt. contg. (9CI)
OTHER NAMES:
CN Estradiol 17-phenylpropionate-estradiol benzoate mixt.
CN Org 369-2
FS STEREOSEARCH
MF C27 H32 O3 . C25 H28 O3
CI MXS
LC STN Files: BIOSIS, CA, CAPLUS, MEDLINE, PHAR, TOXCENTER

CM 1

CRN 26443-03-8
CMF C27 H32 O3

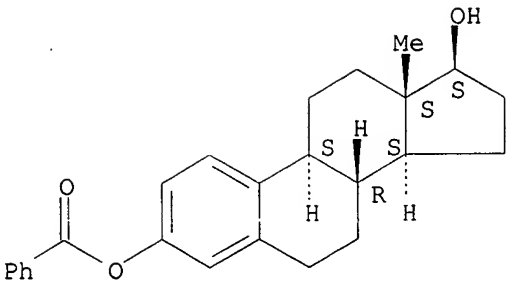
Absolute stereochemistry.



CM 2

CRN 50-50-0
CMF C25 H28 O3

Absolute stereochemistry.



5 REFERENCES IN FILE CA (1962 TO DATE)
5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 94:150845

REFERENCE 2: 94:25592

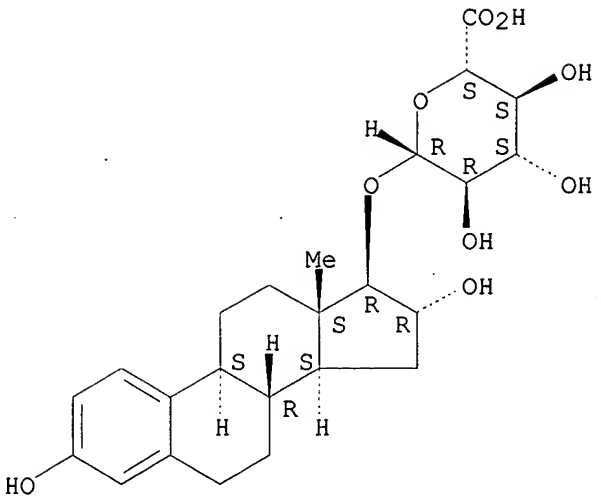
REFERENCE 3: 89:141026

REFERENCE 4: 87:127838

REFERENCE 5: 86:150884

L31 ANSWER 17 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **7219-89-8** REGISTRY
CN .beta.-D-Glucopyranosiduronic acid, (16.alpha.,17.beta.)-3,16-dihydroxyestra-1,3,5(10)-trien-17-yl (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-triene-3,16.alpha.-diol, 17.beta.-(.beta.-D-glucopyranuronosyloxy)- (8CI)
CN Estrane, .beta.-D-glucopyranosiduronic acid deriv.
CN Glucopyranosiduronic acid, 3,16.alpha.-dihydroxyestra-1,3,5(10)-trien-17.beta.-yl, .beta.-D- (7CI, 8CI)
OTHER NAMES:
CN Estriol 17-glucuronide
CN Estriol 17.beta.-(.beta.-D-glucuronide)
CN Estriol 17.beta.-glucuronide
CN Estriol 17.beta.-monoglucuronide
FS STEREOSEARCH
DR 30330-59-7
MF C24 H32 O9
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, DDFU, DRUGU, MEDLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

40 REFERENCES IN FILE CA (1962 TO DATE)
40 REFERENCES IN FILE CAPLUS (1962 TO DATE)
16 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 130:90648

REFERENCE 2: 128:124540

REFERENCE 3: 127:215349

REFERENCE 4: 127:14340

REFERENCE 5: 125:168536

REFERENCE 6: 121:103306

REFERENCE 7: 120:134902

REFERENCE 8: 111:71163

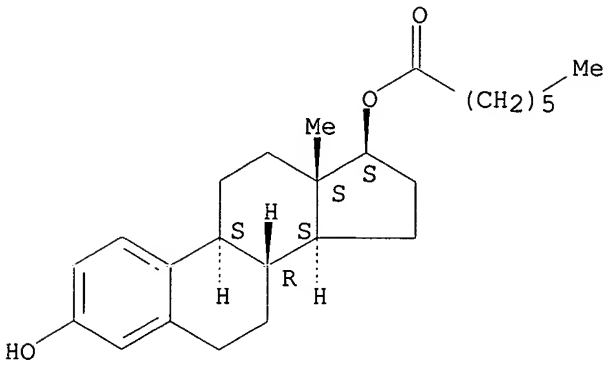
REFERENCE 9: 108:216410

REFERENCE 10: 108:183063

L31 ANSWER 18 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **4956-37-0** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-heptanoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol, 17-heptanoate (6CI, 7CI, 8CI)
CN Heptanoic acid, 3-hydroxyestra-1,3,5(10)-trien-17.beta.-yl ester (8CI)
OTHER NAMES:
CN Estradiol 17-enanthate
CN Estradiol enanthate
CN SQ 16150
FS STEREOSEARCH
MF C25 H36 O3
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD,

CAPLUS, CHEMCATS, CHEMLIST, CSCHEM, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

37 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
37 REFERENCES IN FILE CAPLUS (1962 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:61309

REFERENCE 2: 132:156865

REFERENCE 3: 128:119651

REFERENCE 4: 127:243636

REFERENCE 5: 126:312415

REFERENCE 6: 125:230857

REFERENCE 7: 124:165486

REFERENCE 8: 117:219834

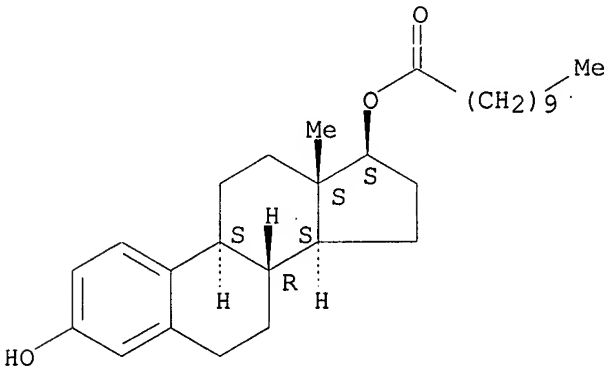
REFERENCE 9: 112:151977

REFERENCE 10: 109:223419

L31 ANSWER 19 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **3571-53-7** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-undecanoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol, 17-undecanoate (7CI, 8CI)
OTHER NAMES:
CN Delestrec
CN Depogin
CN Estradiol 17-undecylate

CN Estradiol undecylate
CN Oestradiol undecylate
CN SQ 9993
FS STEREOSEARCH
DR 349533-54-6
MF C29 H44 O3
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CHEMLIST, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

27 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
27 REFERENCES IN FILE CAPLUS (1962 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:111953

REFERENCE 2: 129:170510

REFERENCE 3: 128:119651

REFERENCE 4: 127:243636

REFERENCE 5: 117:219834

REFERENCE 6: 109:223419

REFERENCE 7: 95:109222

REFERENCE 8: 90:98154

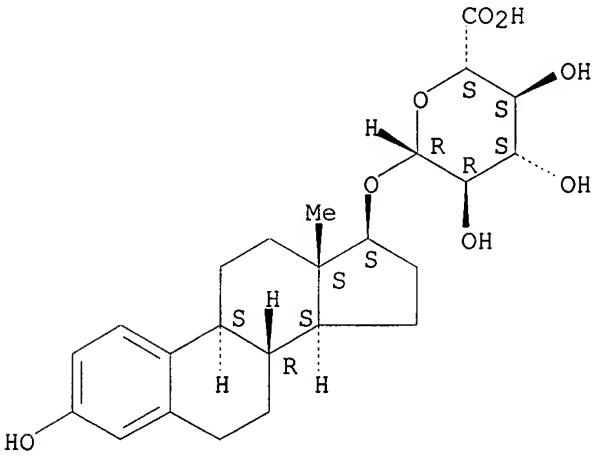
REFERENCE 9: 89:40000

REFERENCE 10: 86:96005

L31 ANSWER 20 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **1806-98-0** REGISTRY

CN .beta.-D-Glucopyranosiduronic acid, (17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estrane, .beta.-D-glucopyranosiduronic acid deriv.
CN Glucopyranosiduronic acid, 3-hydroxyestra-1,3,5(10)-trien-17.beta.-yl, .beta.-D- (6CI, 7CI, 8CI)
OTHER NAMES:
CN Estradiol 17-glucuronide
CN Estradiol 17.beta.-(.beta.-D-glucuronide)
CN Estradiol 17.beta.-glucuronide
FS STEREOSEARCH
DR 125926-20-7, 27851-73-6, 30137-07-6
MF C24 H32 O8
CI COM
LC STN Files: BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, DDFU, DRUGU, EMBASE, IPA, MEDLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

282 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
282 REFERENCES IN FILE CAPLUS (1962 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:233593

REFERENCE 2: 138:198339

REFERENCE 3: 138:185582

REFERENCE 4: 138:184677

REFERENCE 5: 138:102166

REFERENCE 6: 138:49551

REFERENCE 7: 138:16340

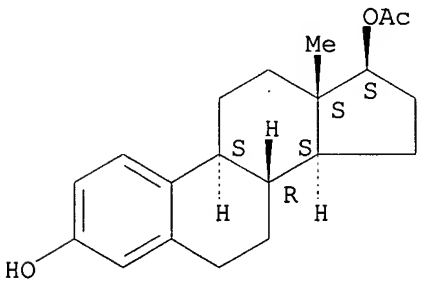
REFERENCE 8: 138:11194

REFERENCE 9: 138:2713

REFERENCE 10: 138:1537

L31 ANSWER 21 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **1743-60-8** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-acetate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol, 17-acetate (6CI, 7CI, 8CI)
OTHER NAMES:
CN .beta.-Estradiol 17-acetate
CN 17.beta.-Acetylestradiol
CN 17.beta.-Estradiol 17-acetate
CN Estra-1,3,5(10)-triene-3,17.beta.-diol 17-acetate
CN Estradiol 17-monoacetate
FS STEREOSEARCH
MF C20 H26 O3
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, EMBASE, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

120 REFERENCES IN FILE CA (1962 TO DATE)
121 REFERENCES IN FILE CAPLUS (1962 TO DATE)
17 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:226330

REFERENCE 2: 138:214660

REFERENCE 3: 138:204502

REFERENCE 4: 138:197926

REFERENCE 5: 138:66804

REFERENCE 6: 138:61161

REFERENCE 7: 137:114053

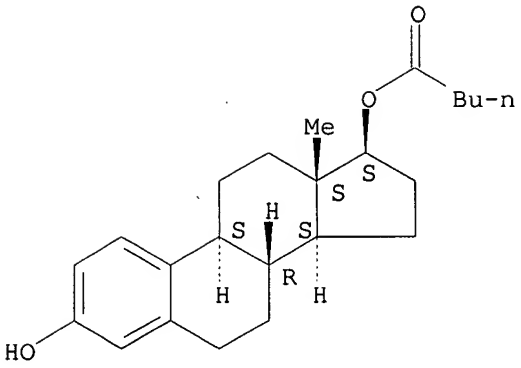
REFERENCE 8: 136:161485

REFERENCE 9: 136:24784

REFERENCE 10: 135:268418

L31 ANSWER 22 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **979-32-8** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-pentanoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol valerate (6CI)
CN Estradiol, 17-valerate (7CI, 8CI)
OTHER NAMES:
CN 3-Hydroxy-17.beta.-valeroyloxyestra-1,3,5(10)-triene
CN Atladiol
CN Climaval
CN Deladiol
CN Delahormone unimatic
CN Delestrogen
CN Delestrogen 4x
CN Dura-Estradiol
CN Estra-1,3,5(10)-triene-3,17.beta.-diol 17-valerate
CN Estradiol 17.beta.-valerate
CN Estradiol valerianate
CN Estraval
CN Femogex
CN Gynogen LA
CN Gynogen LA 40
CN Neofollin
CN NSC 17590
CN Nuvelle
CN Oestradiol valerinate
CN Pelanin Depot
CN Pharlon
CN Primofol-Depot
CN Primogyn-Depot
CN Progynon-Depot
CN Progynova
CN Valergen
FS STEREOSEARCH
DR 907-12-0, 69557-95-5
MF C23 H32 O3
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CBNB, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, NIOSHTIC, PHARMASEARCH, PROMT, RTECS*, TOXCENTER, ULIDAT, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

777 REFERENCES IN FILE CA (1962 TO DATE)
8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
778 REFERENCES IN FILE CAPLUS (1962 TO DATE)
39 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:248709

REFERENCE 2: 138:231902

REFERENCE 3: 138:231901

REFERENCE 4: 138:158871

REFERENCE 5: 138:146907

REFERENCE 6: 138:101107

REFERENCE 7: 138:83614

REFERENCE 8: 138:33532

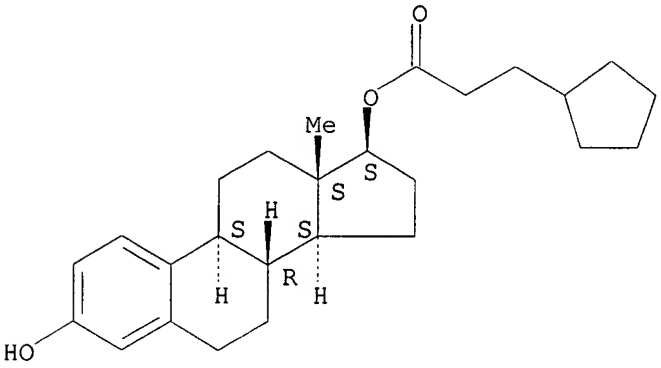
REFERENCE 9: 137:363705

REFERENCE 10: 137:346927

L31 ANSWER 23 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **313-06-4** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-cyclopentanepropanoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cyclopentanepropionic acid, 3-hydroxyestra-1,3,5(10)-trien-17.beta.-yl ester (8CI)
CN Estradiol, 17-cyclopentanepropionate (6CI, 7CI, 8CI)
OTHER NAMES:
CN 17.beta.-Estradiol 17-cyclopentylpropionate
CN Cyclopentanepropionic acid, 17-ester with estradiol
CN Depgynogen
CN Depo-Estradiol
CN Depo-estradiol cyclopentylpropionate
CN Depoestradiol
CN Depoestradiol cypionate
CN Depofemin
CN ECP
CN Estradep

CN Estradiol 17-cyclopentylpropionate
CN Estradiol 17-cypionate
CN Estradiol 17.beta.-cyclopentanepropionate
CN Estradiol 17.beta.-cyclopentylpropionate
CN Estradiol 17.beta.-cypionate
CN Estradiol cyclopentylpropionate
CN Estradiol cypionate
FS STEREOSEARCH
MF C26 H36 O3
CI COM
LC STN Files: ADISNEWS, AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IPA, MEDLINE, MRCK*, NIOSHTIC, PROMT, RTECS*, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

239 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
239 REFERENCES IN FILE CAPLUS (1962 TO DATE)
23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:248694

REFERENCE 2: 138:61309

REFERENCE 3: 138:420

REFERENCE 4: 136:330639

REFERENCE 5: 136:257418

REFERENCE 6: 136:189473

REFERENCE 7: 136:48588

REFERENCE 8: 135:376767

REFERENCE 9: 135:376764

REFERENCE 10: 135:348976

L31 ANSWER 24 OF 24 REGISTRY COPYRIGHT 2003 ACS
RN **57-63-6** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Nor-17.alpha.-pregna-1,3,5(10)-trien-20-yne-3,17-diol (6CI, 7CI, 8CI)
OTHER NAMES:
CN 17-Ethinyl-3,17-estradiol
CN 17-Ethinylestradiol
CN 17-Ethynyl-3,17-dihydroxy-1,3,5-oestratriene
CN 17-Ethynylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17-Ethynylestradiol
CN 17-Nor-17.alpha.-pregna-1,3,5-(10)-trien-20-yne-3,17-diol
CN 17.alpha.-Ethinyl-1,3,5(10)-estratriene-3,17-diol
CN 17.alpha.-Ethinyl-17.beta.-estradiol
CN 17.alpha.-Ethinyl-3,17-dihydroxy-.DELTA.1,3,5-estratriene
CN 17.alpha.-Ethinylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17.alpha.-Ethinylestradiol
CN 17.alpha.-Ethynylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17.alpha.-Ethynylestradiol
CN 19-Nor-17.alpha.-pregna-1,3,5(10)-trien-20-yne-3,17.beta.-diol
CN Amenoron
CN Chee-O-Gen
CN Chee-O-Genf
CN Diogyn E
CN Dyloform
CN Esteed
CN Estigyn
CN Estinyl
CN Eston-E
CN Estoral
CN Estorals
CN Estradiol, 17-ethynyl-
CN Ethidol
CN Ethinoral
CN Ethinylestradiol
CN Ethinyloestradiol
CN Ethynylestradiol
CN Ethynyloestradiol
CN Eticyclin
CN Eticyclol
CN Etinestrol
CN Etinestryl
CN Etinoestryl
CN Etistradiol
CN Follicoral
CN Ginestrene
CN Inestra
CN Linoral
CN Lynoral
CN Menolyn
CN Microfollin
CN neo-Estrone
CN Novestrol
CN NSC 10973
CN Oradiol
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY
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DR 77538-56-8, 406932-93-2
MF C20 H24 O2
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,

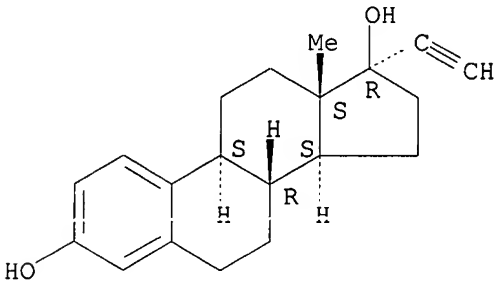
BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DIOGENES, DRUGNL, DRUGU, DRUGUPDATES, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PHAR, PROMT, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VETU

(*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**, WHO

(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3971 REFERENCES IN FILE CA (1962 TO DATE)
80 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3974 REFERENCES IN FILE CAPLUS (1962 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:260224

REFERENCE 2: 138:259542

REFERENCE 3: 138:259505

REFERENCE 4: 138:255252

REFERENCE 5: 138:250058

REFERENCE 6: 138:248696

REFERENCE 7: 138:248678

REFERENCE 8: 138:248673

REFERENCE 9: 138:248406

REFERENCE 10: 138:243401

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 19:50:06 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 22 Apr 2003  VOL 138 ISS 17
FILE LAST UPDATED: 21 Apr 2003  (20030421/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L3          8197 SEA FILE=REGISTRY SSS FUL L1
L4             STR
L5             STR
L6             STR
L7             STR
L8          4034 SEA FILE=REGISTRY SUB=L3 SSS FUL L1 NOT (L4 OR L5 OR L6 OR L7)
L15            STR
L16            5 SEA FILE=REGISTRY SUB=L3 SSS FUL L15
L17           37 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16
L19         4034 SEA FILE=REGISTRY ABB=ON  PLU=ON  L8 NOT L16
L20         8877 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L21            2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)CYTOPROTECT?
L22            2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 NOT L17
L24          357 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L20 AND ?PROTECT?) NOT (L17
                 OR L22)
L27          974 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20(L)(?MEDIC? OR ?THERAP? OR
                 ?DRUG? OR ?PHARM?)
L29           45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND L27
L30           25 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 NOT (2003 OR 2002 OR
                 2001)/PY
L32           20 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 NOT L30


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L32  ANSWER 1 OF 20  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2003:202410  HCAPLUS
DOCUMENT NUMBER:          138:226705
TITLE:                    Novel pharmaceuticals comprising drug conjugates with
                          polypeptide carriers
INVENTOR(S):              Picariello, Thomas
PATENT ASSIGNEE(S):       New River Pharmaceuticals Inc., USA
SOURCE:                   PCT Int. Appl., 2059 pp.
```

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020200	A2	20030313	WO 2001-US43117	20011116

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2000-248600P	P	20001116
US 2000-248601P	P	20001116
US 2000-248603P	P	20001116
US 2000-248604P	P	20001116
US 2000-248606P	P	20001116
US 2000-248607P	P	20001116
US 2000-248608P	P	20001116
US 2000-248609P	P	20001116
US 2000-248611P	P	20001116
US 2000-248689P	P	20001116
US 2000-248691P	P	20001116
US 2000-248692P	P	20001116
US 2000-248693P	P	20001116
US 2000-248694P	P	20001116
US 2000-248695P	P	20001116
US 2000-248696P	P	20001116
US 2000-248697P	P	20001116
US 2000-248698P	P	20001116
US 2000-248701P	P	20001116
US 2000-248702P	P	20001116
US 2000-248703P	P	20001116
US 2000-248704P	P	20001116
US 2000-248705P	P	20001116
US 2000-248706P	P	20001116
US 2000-248707P	P	20001116
US 2000-248708P	P	20001116
US 2000-248709P	P	20001116
US 2000-248710P	P	20001116
US 2000-248711P	P	20001116
US 2000-248712P	P	20001116

IT **57-63-6D**, Ethinyl estradiol, polypeptide conjugates
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel **pharmaceuticals** comprising **drug** conjugates with polypeptide carriers)

L32 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2003:173409 HCAPLUS
DOCUMENT NUMBER: 138:226720
TITLE: Transdermal therapeutic system based on polyacrylate-contact-bonding adhesives without functional groups for the use with steroid hormones and other drugs
INVENTOR(S): Klein, Robert-Peter; Hille, Thomas; Theobald, Frank
PATENT ASSIGNEE(S): LTS Lohmann Therapie-Systeme AG, Germany; Klein, Ursula, Hildegard

SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003017988	A1	20030306	WO 2002-EP9057	20020813
W: AU, BR, CA, CN, JP, KR, MX, US, ZA				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
DE 10141652	A1	20030313	DE 2001-10141652	20010824

PRIORITY APPLN. INFO.: DE 2001-10141652 A 20010824
IT **57-63-6**, Ethynylestradiol
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(transdermal **therapeutic** system based on polyacrylate-contact-bonding adhesives without functional groups for use with steroid hormones and other **drugs**)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:888569 HCAPLUS
DOCUMENT NUMBER: 137:370278
TITLE: Preparation of substituted pregna-1,3,5(10)-triene derivatives for pharmaceutical use
INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
PATENT ASSIGNEE(S): Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092100	A1	20021121	WO 2002-GB2210	20020513
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2001-290013P P 20010511
OTHER SOURCE(S): MARPAT 137:370278
IT **229486-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted pregna-1,3,5(10)-triene derivs. for a variety of **therapeutic** uses)
IT **475486-79-4P 475486-80-7P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted pregna-1,3,5(10)-triene derivs. for a variety of

therapeutic uses)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:822466 HCAPLUS
Correction of: 2002:171950
DOCUMENT NUMBER: 138:1537
Correction of: 136:228584
TITLE: ABC transporter proteins modified in their C-terminal tripeptide motif exhibit improved drug resistance and novel membrane localization
INVENTOR(S): Board, Philip; Harris, Matthew
PATENT ASSIGNEE(S): The Australian National University, Australia
SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018438	A1	20020307	WO 2001-AU1093	20010830
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001085578	A5	20020313	AU 2001-85578	20010830

PRIORITY APPLN. INFO.: US 2000-229663P P 20000831
WO 2001-AU1093 W 20010830

IT **57-63-6**, Ethinylestradiol **1806-98-0**, Estradiol-17.beta.-glucuronide
RL: ADV (Adverse effect, including toxicity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cholestatic agent, resistance to; ABC transporter proteins modified in their C-terminal tripeptide motif exhibit improved **drug** resistance and novel membrane localization)

L32 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:778718 HCAPLUS
DOCUMENT NUMBER: 137:289046
TITLE: Methods and compositions for enhancing pharmaceutical treatments
INVENTOR(S): Newman, Michael J.; Dixon, William Ross
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 47 pp., Cont.-in-part of U.S. Ser. No. 684,293.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002147197	A1	20021010	US 2002-104549	20020320

PRIORITY APPLN. INFO.: US 1999-158322P P 19991008

US 2000-684293 A2 20001006
OTHER SOURCE(S): MARPAT 137:289046
IT **1806-98-0 1806-98-0D**, derivs., analogs, and metabolites
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods and compns. for enhancing **pharmaceutical** treatments)

L32 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:717058 HCAPLUS
DOCUMENT NUMBER: 137:237777
TITLE: Drospirenone for hormone replacement therapy
INVENTOR(S): Heil, Wolfgang; Hilmann, Juergen; Lipp, Ralph; Schuermann, Rolf
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: U.S. Pat. Appl. Publ., 14 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002132801	A1	20020919	US 2001-757688	20010111

PRIORITY APPLN. INFO.: US 2001-757688 20010111
IT **57-63-6**, Ethinyl estradiol **514-68-1**, Estriol succinate **979-32-8**, Estradiol valerate
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(drospirenone for hormone replacement **therapy**)

L32 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:558773 HCAPLUS
DOCUMENT NUMBER: 137:119626
TITLE: Monofluorophosphate combined with hormone replacement therapy in postmenopausal osteoporosis. an open-label pilot efficacy and safety study
AUTHOR(S): Ringe, Johann Diederich; Setnikar, Ivo
CORPORATE SOURCE: Department of Internal Med. IV, Klinikum Leverkusen, Teaching Hospital of the University of Cologne, Leverkusen, Germany
SOURCE: Rheumatology International (2002), 22(1), 27-32
CODEN: RHINDE; ISSN: 0172-8172
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **979-32-8**, Estradiol valerate
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(monofluorophosphate combined with hormone replacement **therapy** in postmenopausal osteoporosis)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:223517 HCAPLUS
DOCUMENT NUMBER: 136:335402
TITLE: Intrauterine 10.mu.g and 20.mu.g levonorgestrel systems in postmenopausal women receiving oral oestrogen replacement therapy: clinical, endometrial and metabolic response
AUTHOR(S): Raudaskoski, T.; Tapanainen, J.; Tomas, E.; Luotola, H.; Pekonen, F.; Ronni-Sivula, H.; Timonen, H.;

Riphagen, F.; Laatikainen, T.
CORPORATE SOURCE: Department of Obstetries and Gynecology, Oulu University Hospital, Oulu, 90029, Finland
SOURCE: BJOG (2002), 109(2), 136-144
CODEN: BIOGFQ
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **979-32-8**, Progynova
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(intrauterine 10.mu.g and 20.mu.g levonorgestrel systems in postmenopausal women receiving oral estrogen replacement **therapy**)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:171950 HCAPLUS
DOCUMENT NUMBER: 136:228584
TITLE: ABC transporter proteins modified in their C-terminal tripeptide motif exhibit improved drug resistance and novel membrane localization
INVENTOR(S): Board, Philip; Harris, Matthew
PATENT ASSIGNEE(S): The Australian National University, Australia
SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018438 A1		20020307	WO 2001-AU1093	20010830

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR

PRIORITY APPLN. INFO.: US 2000-PV229663 20000831
IT **57-63-6**, Ethinylestradiol **1806-98-0**, Estradiol-17.beta.-glucuronide
RL: ADV (Adverse effect, including toxicity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cholestatic agent, resistance to; ABC transporter proteins modified in their C-terminal tripeptide motif exhibit improved **drug** resistance and novel membrane localization)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:798083 HCAPLUS
DOCUMENT NUMBER: 135:362557
TITLE: Flavopiridol drug combinations and methods with reduced side effects
INVENTOR(S): Ratain, Mark J.; Innocenti, Federico; Iyer, Lalitha
PATENT ASSIGNEE(S): Arch Development Corporation, USA
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001080896	A2	20011101	WO 2001-US12526	20010412
WO 2001080896	A3	20020711		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-553829 A1 20000421
IT **1806-98-0 371755-19-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(flavopiridol **drug** combinations and methods with reduced side effects)

L32 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:678574 HCAPLUS
DOCUMENT NUMBER: 136:79948
TITLE: Hormone replacement therapy may improve hepatic function in women with Turner's syndrome
AUTHOR(S): Elsheikh, M.; Hodgson, H. J. F.; Wass, J. A. H.; Conway, G. S.
CORPORATE SOURCE: Department of Endocrinology, Radcliffe Infirmary, Oxford, UK
SOURCE: Clinical Endocrinology (Oxford, United Kingdom) (2001), 55(2), 227-231
CODEN: CLECAP; ISSN: 0300-0664
PUBLISHER: Blackwell Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **979-32-8**, Estradiol valerate
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hormone replacement **therapy** effect on hepatic function in women with Turner's syndrome)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:661646 HCAPLUS
DOCUMENT NUMBER: 135:205582
TITLE: Caspase inhibitory factor (CIF), screening method, and therapeutic methods
INVENTOR(S): Leblanc, Andrea
PATENT ASSIGNEE(S): McGill University, Can.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001064937	A2	20010907	WO 2001-CA210	20010221	
WO 2001064937	A3	20020207			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
EP 1259637	A2	20021127	EP 2001-909367	20010221	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
PRIORITY APPLN. INFO.:			US 2000-186330P	P	20000302
			WO 2001-CA210	W	20010221

IT **57-63-6**, Ethinyl estradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(caspase inhibitory factor (CIF), screening method, and **therapeutic** methods)

L32 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:545492 HCAPLUS
DOCUMENT NUMBER: 135:127209
TITLE: Pharmaceutical compositions containing drospirenone for hormone replacement therapy
INVENTOR(S): Heil, Wolfgang; Hilmann, Juergen; Lipp, Ralph; Schuermann, Rolf
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 2001052857	A1	20010726	WO 2001-IB41	20010118	
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
BR 2001007683	A	20021112	BR 2001-7683	20010118	
EP 1257280	A1	20021120	EP 2001-900579	20010118	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
NO 2002002966	A	20020918	NO 2002-2966	20020620	
PRIORITY APPLN. INFO.:			EP 2000-200183	A	20000118
			US 2000-484026	A	20000118
			WO 2001-IB41	W	20010118

IT **164017-31-6 350818-74-5 350818-78-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(**pharmaceutical** compns. contg. drospirenone and estrogen for treatment of diseases, disorders, and symptoms assocd. with deficient estrogen levels)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:338762 HCAPLUS
DOCUMENT NUMBER: 134:362292
TITLE: Methods of determining individual hypersensitivity to a pharmaceutical agent from gene expression profile
INVENTOR(S): Farr, Spencer
PATENT ASSIGNEE(S): Phase-1 Molecular Toxicology, USA
SOURCE: PCT Int. Appl., 222 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032928	A2	20010510	WO 2000-US30474	20001103
WO 2001032928	A3	20020725		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-165398P P 19991105
US 2000-196571P P 20000411

IT **79871-54-8**, Norgestimate-ethinyl estradiol mixt.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Norgestimate/ethinyl estradiol; methods of detg. individual hypersensitivity to a **pharmaceutical** agent from gene expression profile)
IT **57-63-6**, Ethinyl estradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(methods of detg. individual hypersensitivity to a **pharmaceutical** agent from gene expression profile)
IT **8056-51-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods of detg. individual hypersensitivity to a **pharmaceutical** agent from gene expression profile)

L32 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:819400 HCAPLUS
DOCUMENT NUMBER: 132:64448
TITLE: Preparation of 17-halogenated 19-nor steroids as antitumor and antiosteoporotic agents
INVENTOR(S): Bouali, Yasmina; Mauger, Jacques; Nique, Francois; Van De Velde, Patrick
PATENT ASSIGNEE(S): Hoechst Marion Roussel, Fr.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9967274	A1	19991229	WO 1999-FR1491	19990622
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2780060	A1	19991224	FR 1998-7898	19980623
FR 2780060	B1	20000804		
CA 2336167	AA	19991229	CA 1999-2336167	19990622
AU 9942705	A1	20000110	AU 1999-42705	19990622
BR 9912206	A	20010410	BR 1999-12206	19990622
EP 1090027	A1	20010411	EP 1999-957166	19990622
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002518516	T2	20020625	JP 2000-555925	19990622
NZ 508535	A	20020828	NZ 1999-508535	19990622
NO 2000006573	A	20010222	NO 2000-6573	20001221
US 6423700	B1	20020723	US 2001-720565	20010105
US 2003022874	A1	20030130	US 2002-173914	20020618

PRIORITY APPLN. INFO.:
FR 1998-7898 A 19980623
WO 1999-FR1491 W 19990622
US 2001-720565 A3 20010105

OTHER SOURCE(S): MARPAT 132:64448
IT **253169-29-8P 253169-30-1P 253169-31-2P**
253169-32-3P 253169-33-4P 253169-34-5P
253169-35-6P 253169-36-7P 253169-40-3P
253169-41-4P 253169-42-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and **pharmaceutical** compns. of 17-halogenated 19-nor steroids)
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:13846 HCAPLUS
DOCUMENT NUMBER: 128:93195
TITLE: Transdermal pharmaceuticals containing two active principles in separate compartments
INVENTOR(S): Dubois, Jean-Luc
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.; Dubois, Jean-Luc
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9747305	A1	19971218	WO 1997-FR1024	19970610
W: AU, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, PL, RU, TR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2749514	A1	19971212	FR 1996-7209	19960611

FR 2749514	B1	19980807			
CA 2257913	AA	19971218	CA 1997-2257913		19970610
AU 9732661	A1	19980107	AU 1997-32661		19970610
AU 739141	B2	20011004			
EP 904086	A1	19990331	EP 1997-928318		19970610
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
CN 1227492	A	19990901	CN 1997-197162		19970610
JP 2000511921	T2	20000912	JP 1998-501289		19970610
ZA 9705160	A	19980611	ZA 1997-5160		19970611
NO 9805807	A	19990210	NO 1998-5807		19981211
KR 2000016582	A	20000325	KR 1998-710177		19981211
PRIORITY APPLN. INFO.:			FR 1996-7209	A	19960611
			WO 1997-FR1024	W	19970610

IT **57-63-6**, Ethynyl estradiol
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(transdermal **pharmaceuticals** contg. two active principles in sep. compartments)

L32 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:626237 HCAPLUS
DOCUMENT NUMBER: 119:226237
TITLE: Preparation of estrogen bisphosphonates for treatment of bone disease
INVENTOR(S): Sugioka, Tatsuo; Inazu, Mizuho
PATENT ASSIGNEE(S): Hoechst Japan Ltd., Japan
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 548884	A1	19930630	EP 1992-121707		19921221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
JP 05230086	A2	19930907	JP 1992-311876		19921120
JP 3141053	B2	20010305			
CA 2086026	AA	19930627	CA 1992-2086026		19921222
US 5428181	A	19950627	US 1992-996596		19921224
PRIORITY APPLN. INFO.:			JP 1991-344253	A	19911226
			JP 1992-311876	A	19921120

OTHER SOURCE(S): MARPAT 119:226237
IT **88899-72-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepn. of **drug** for treatment of bone disease)

L32 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:574681 HCAPLUS
DOCUMENT NUMBER: 115:174681
TITLE: Preparation of steroid enzyme inhibitors for treatment of benign prostatic hyperplasia
INVENTOR(S): Labrie, Fernand
PATENT ASSIGNEE(S): Endorecherche Inc., Can.
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9100731	A1	19910124	WO 1990-CA210	19900705
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
CA 2062973	AA	19910108	CA 1990-2062973	19900705
AU 9058545	A1	19910206	AU 1990-58545	19900705
AU 643445	B2	19931118		
EP 480950	A1	19920422	EP 1990-909598	19900705
EP 480950	B1	19990324		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
HU 60138	A2	19920828	HU 1992-47	19900705
JP 04506798	T2	19921126	JP 1990-509262	19900705
JP 3332377	B2	20021007		
EP 857487	A2	19980812	EP 1998-104849	19900705
EP 857487	A3	19991208		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
AT 177949	E	19990415	AT 1990-909598	19900705
ES 2133270	T3	19990916	ES 1990-909598	19900705
EP 943328	A2	19990922	EP 1999-106510	19900705
EP 943328	A3	19991208		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 2001354590	A2	20011225	JP 2001-177144	19900705
ZA 9005312	A	19920226	ZA 1990-5312	19900706
IL 94990	A1	19970110	IL 1990-94990	19900706
AU 9352174	A1	19940210	AU 1993-52174	19931203
AU 668434	B2	19960502		
US 5595985	A	19970121	US 1993-167450	19931215
US 5817649	A	19981006	US 1995-476933	19950607
US 6423698	B1	20020723	US 1995-484461	19950607

PRIORITY APPLN. INFO.:

US 1989-376700	A	19890707
US 1989-322154	B2	19890310
EP 1990-909598	A3	19900705
EP 1998-104849	A3	19900705
JP 1990-509262	A3	19900705
WO 1990-CA210	A	19900705
US 1992-925883	B1	19920806
US 1993-167450	A3	19931215

IT **98008-57-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of prostatic hyperplasia **drug**)

L32 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:485452 HCAPLUS
DOCUMENT NUMBER: 115:85452
TITLE: Preparation of steroidal enzyme inhibitors for treatment of prostate cancer
INVENTOR(S): Labrie, Fernand
PATENT ASSIGNEE(S): Endorecherche Inc., Can.
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9100733	A1	19910124	WO 1990-CA212	19900705
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				

RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE

CA 2062792	AA	19910108	CA 1990-2062792	19900705
AU 9058516	A1	19910206	AU 1990-58516	19900705
HU 60139	A2	19920828	HU 1992-48	19900705
JP 04506799	T2	19921126	JP 1990-509263	19900705
JP 3350048	B2	20021125		
EP 595796	A1	19940511	EP 1990-909601	19900705
EP 595796	B1	20030115		

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE

AT 230994	E	20030215	AT 1990-909601	19900705
ZA 9005313	A	19920226	ZA 1990-5313	19900706
IL 94991	A1	19991130	IL 1990-94991	19900706
US 5372996	A	19941213	US 1992-963278	19921019
US 5593981	A	19970114	US 1993-98607	19930910
AU 9463425	A1	19940721	AU 1994-63425	19940530
AU 665311	B2	19951221		
US 5610150	A	19970311	US 1995-472512	19950607

PRIORITY APPLN. INFO.:	US 1989-376710	A	19890707
	US 1989-322154	B2	19890310
	WO 1990-CA212	A	19900705
	US 1992-963278	A3	19921019
	US 1993-98607	A3	19930910

OTHER SOURCE(S): MARPAT 115:85452

IT **98008-57-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of **drug** for prostate cancer treatment)

L32 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1988:597190 HCAPLUS
DOCUMENT NUMBER:	109:197190
TITLE:	Combination dosage form containing estrogens and progestogens for pre-menopausal women
INVENTOR(S):	Upton, Gertrude Virginia
PATENT ASSIGNEE(S):	American Home Products Corp., USA
SOURCE:	Eur. Pat. Appl., 9 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 253607	A1	19880120	EP 1987-306174	19870713
EP 253607	B1	19920429		
EP 253607	B2	20010523		

R: AT, BE, CH, DE, ES, FR, GR, IT, LI, LU, NL, SE

DK 8703518	A	19880116	DK 1987-3518	19870708
AU 8775379	A1	19880121	AU 1987-75379	19870709
AU 597084	B2	19900524		
ZA 8705010	A	19890222	ZA 1987-5010	19870709
WO 8800469	A1	19880128	WO 1987-US1646	19870710

W: JP, KR

JP 01500431	T2	19890216	JP 1987-504480	19870710
JP 2645510	B2	19970825		
GB 2192542	A1	19880120	GB 1987-16431	19870713
GB 2192542	B2	19900502		
AT 75401	E	19920515	AT 1987-306174	19870713
ES 2033850	T3	19930401	ES 1987-306174	19870713

PRIORITY APPLN. INFO.:	US 1986-885971	A	19860715
	WO 1987-US1646	W	19870710

EP 1987-306174 A 19870713

IT **57-63-6**, Ethinyl estradiol
RL: BIOL (Biological study)
(**pharmaceutical** pack contg. progestogen and, for hormonal replacement and contraception)

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HIGHEST E# ASSIGNED. SELECT NOT VALID.

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=> select hit rn l32 1-20
E1 THROUGH E26 ASSIGNED

=> fil reg
FILE 'REGISTRY' ENTERED AT 19:52:10 ON 22 APR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9
DICTIONARY FILE UPDATES: 21 APR 2003 HIGHEST RN 503584-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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1 1806-98-0/BI
(1806-98-0/RN)
1 979-32-8/BI
(979-32-8/RN)
1 98008-57-2/BI
(98008-57-2/RN)
1 164017-31-6/BI
(164017-31-6/RN)
1 229486-17-3/BI
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                1 8056-51-7/BI
                  (8056-51-7/RN)
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                  (88899-72-3/RN)
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                  164017-31-6/BI OR 229486-17-3/BI OR 253169-29-8/BI OR 253169-30-
                  1/BI OR 253169-31-2/BI OR 253169-32-3/BI OR 253169-33-4/BI OR
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                  3/BI OR 253169-41-4/BI OR 253169-42-5/BI OR 350818-74-5/BI OR
                  350818-78-9/BI OR 371755-19-0/BI OR 475486-79-4/BI OR 475486-80-
                  7/BI OR 514-68-1/BI OR 79871-54-8/BI OR 8056-51-7/BI OR 88899-72
                  -3/BI)

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L33  ANSWER 1 OF 26  REGISTRY  COPYRIGHT 2003 ACS
RN   475486-80-7  REGISTRY
CN   Acetamide, N-[(20S)-3-hydroxy-2-methoxy-20-methyl-19-norpregna-1,3,5(10)-
     trien-21-yl]- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C24 H35 N O3
SR   CA
LC   STN Files:   CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
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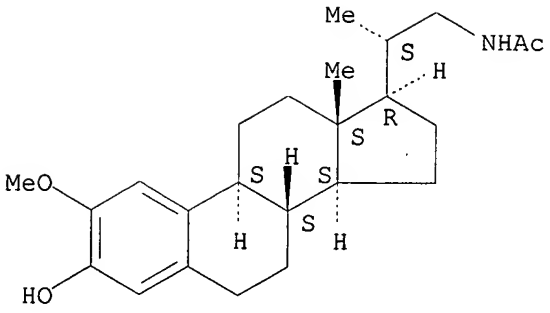


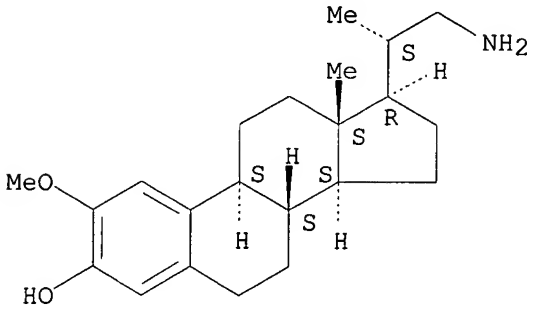
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:370278

L33 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **475486-79-4** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 21-amino-2-methoxy-20-methyl-, (20S)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H33 N O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



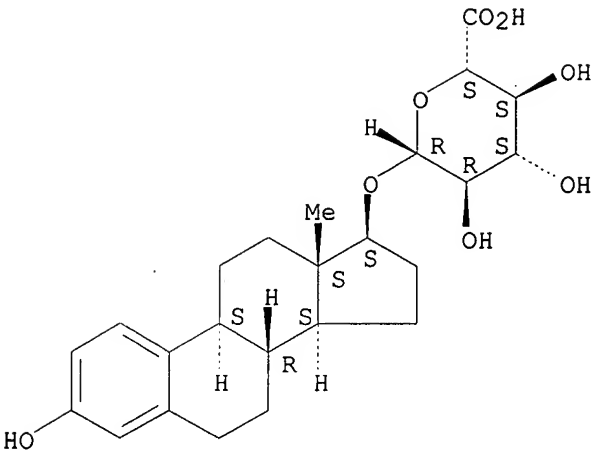
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:370278

L33 ANSWER 3 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **371755-19-0** REGISTRY
CN .beta.-D-Glucopyranosiduronic acid, (17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl, labeled with tritium (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H32 O8
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
IL XH-3

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

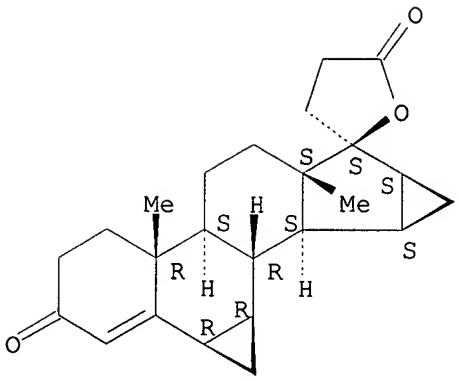
REFERENCE 1: 135:362557

L33 ANSWER 4 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **350818-78-9** REGISTRY
CN Estra-1,3,5(10)-triene-3,16,17-triol, 16,17-bis(hydrogen butanedioate), (16.alpha.,17.beta.)-, mixt. with (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethylspiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Spiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione, 1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethyl-, (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-, mixt. contg. (9CI)
FS STEREOSEARCH
MF C26 H32 O9 . C24 H30 O3
CI MXS
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 67392-87-4
CMF C24 H30 O3

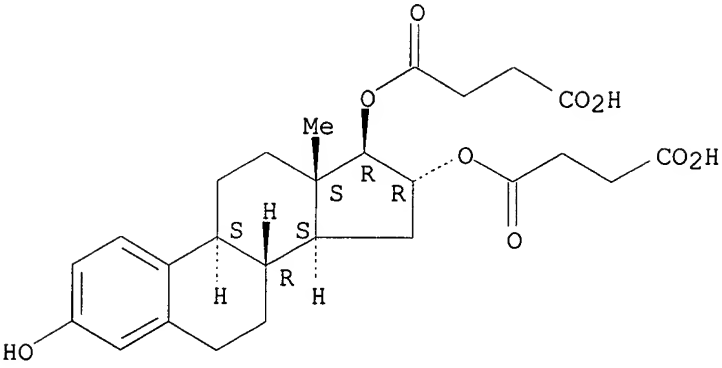
Absolute stereochemistry.



CM 2

CRN 514-68-1
CMF C26 H32 O9

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

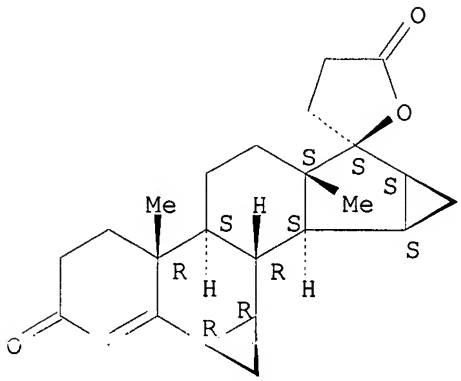
REFERENCE 1: 135:127209

L33 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **350818-74-5** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-pentanoate, mixt. with (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethylspiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Spiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione, 1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethyl-, (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-, mixt. contg. (9CI)
FS STEREOSEARCH
MF C24 H30 O3 . C23 H32 O3
CI MXS
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 67392-87-4
CMF C24 H30 O3

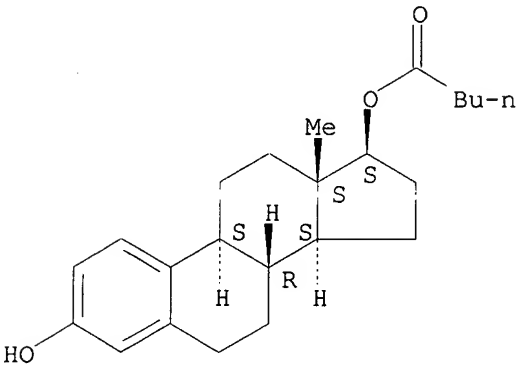
Absolute stereochemistry.



CM 2

CRN 979-32-8
CMF C23 H32 O3

Absolute stereochemistry.

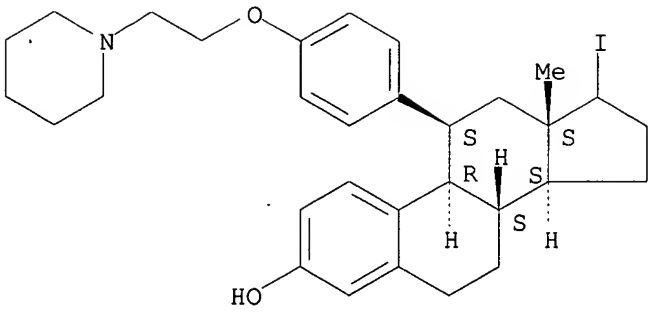


1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:127209

L33 ANSWER 6 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-42-5** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-iodo-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride, (11.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 I N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (253169-34-5)

Absolute stereochemistry.



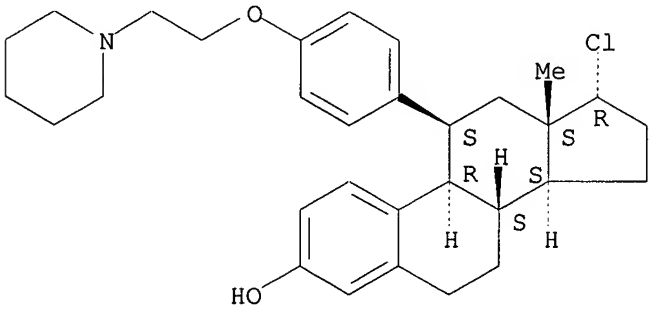
● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 7 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-41-4** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-chloro-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 Cl N O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



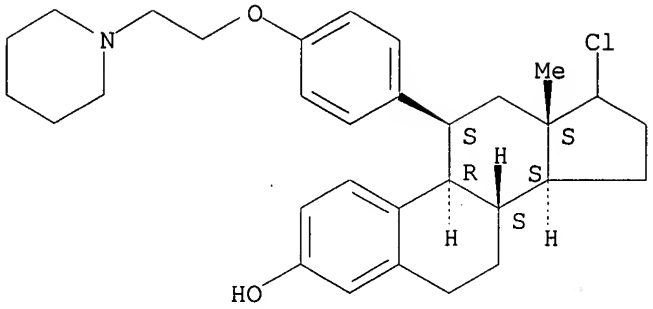
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-40-3** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-chloro-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 Cl N O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



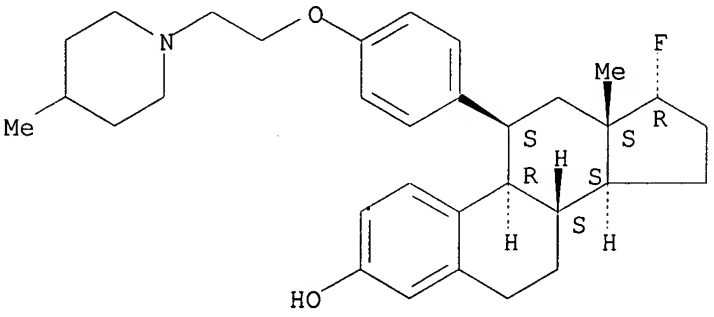
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-36-7** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-fluoro-11-[4-[2-(4-methyl-1-piperidinyl)ethoxy]phenyl]-, hydrochloride, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H42 F N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (253169-35-6)

Absolute stereochemistry.



● HCl

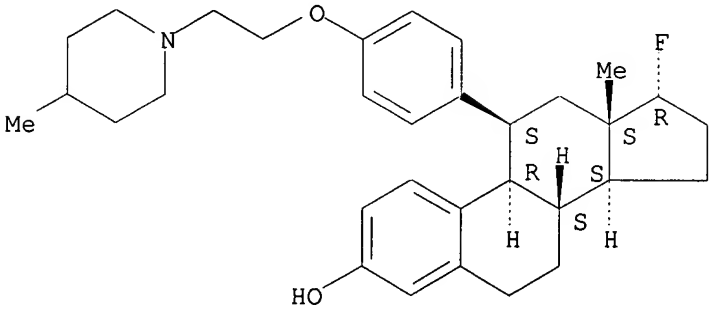
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 10 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-35-6** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-fluoro-11-[4-[2-(4-methyl-1-piperidinyl)ethoxy]phenyl]-, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C32 H42 F N O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



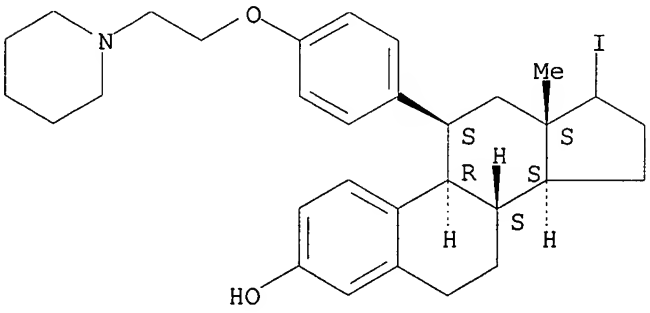
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-34-5** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-iodo-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 I N O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

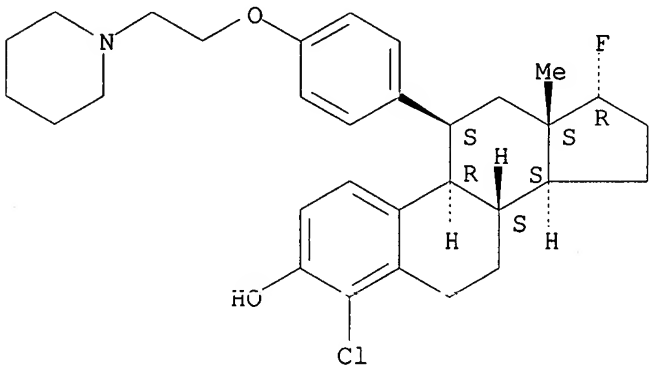
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-33-4** REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 4-chloro-17-fluoro-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H39 Cl F N O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



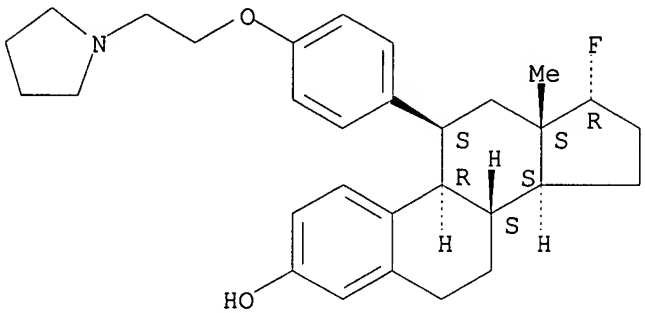
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-32-3** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-fluoro-11-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]-, hydrochloride, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H38 F N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



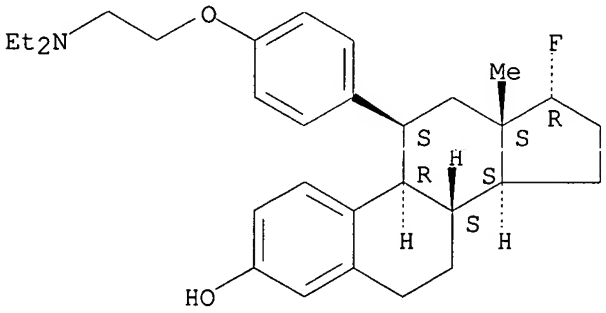
● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 14 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-31-2** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 11-[4-[2-(diethylamino)ethoxy]phenyl]-17-fluoro-, hydrochloride, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H40 F N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



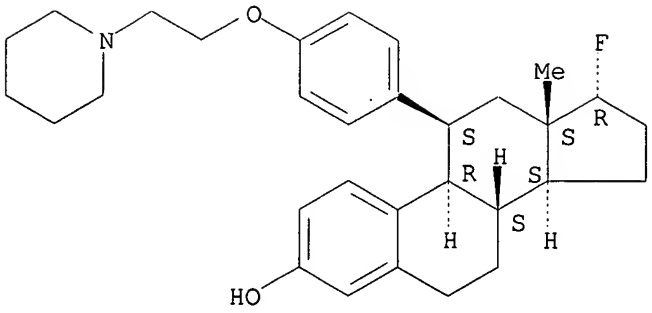
● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 15 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-30-1** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-fluoro-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 F N O2 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (253169-29-8)

Absolute stereochemistry.



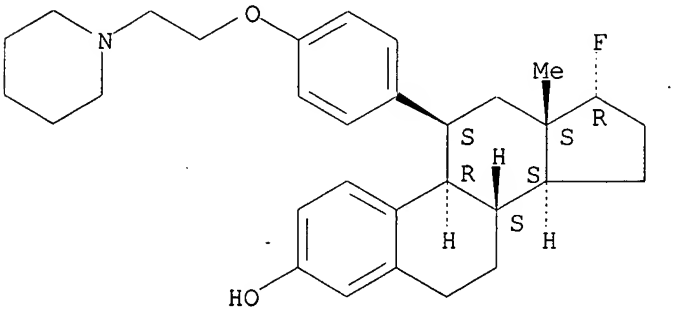
● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 16 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **253169-29-8** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-fluoro-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11.beta.,17.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H40 F N O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

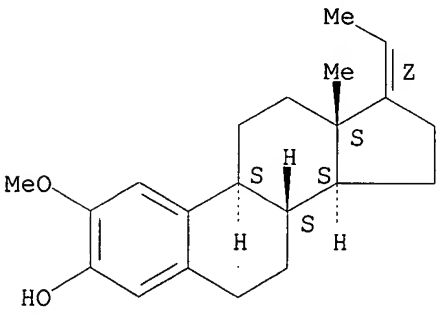
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:64448

L33 ANSWER 17 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **229486-17-3** REGISTRY
CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O2
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:370278

REFERENCE 2: 135:358085

REFERENCE 3: 133:350395

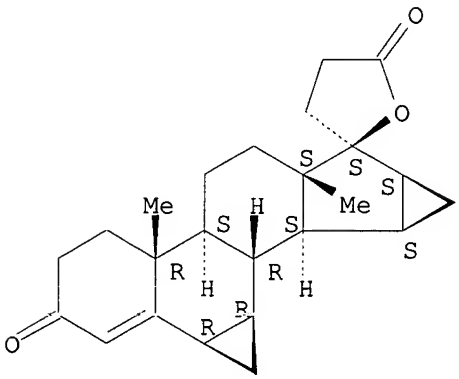
REFERENCE 4: 131:88083

L33 ANSWER 18 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **164017-31-6** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)-, mixt. with (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethylspiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)-, mixt. with [6R-(6.alpha.,7.alpha.,8.beta.,9.alpha.,10.beta.,13.beta.,14.alpha.,15.alpha.,16.alpha.,17.beta.)]-1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethylspiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione
CN Spiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione, 1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethyl-, [6R-(6.alpha.,7.alpha.,8.beta.,9.alpha.,10.beta.,13.beta.,14.alpha.,15.alpha.,16.alpha.,17.beta.)]-, mixt. contg.
CN Spiro[17H-dicyclopropa[6,7:15,16]cyclopenta[a]phenanthrene-17,2'(5'H)-furan]-3,5'(2H)-dione, 1,3',4',6,7,8,9,10,11,12,13,14,15,16,20,21-hexadecahydro-10,13-dimethyl-, (2'S,6R,7R,8R,9S,10R,13S,14S,15S,16S)-, mixt. contg. (9CI)
OTHER NAMES:
CN Drospirenone-ethinylestradiol mixt.
CN Ethinylestradiol-drospirenone mixt.
CN Yasmin
FS STEREOSEARCH
MF C24 H30 O3 . C20 H24 O2
CI MXS
SR CA
LC STN Files: BIOSIS, BIOTECHNO, CA, CAPLUS, CIN, DIOGENES, DRUGPAT, DRUGUPDATES, EMBASE, PROMT, TOXCENTER, USPATFULL

CM 1

CRN 67392-87-4
CMF C24 H30 O3

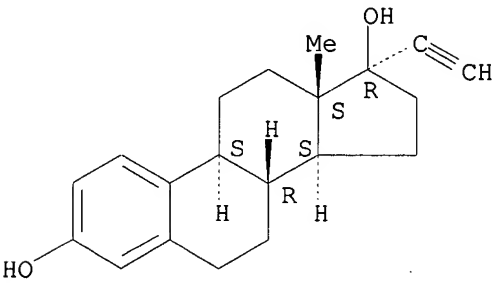
Absolute stereochemistry.



CM 2

CRN 57-63-6
CMF C20 H24 O2

Absolute stereochemistry.



18 REFERENCES IN FILE CA (1962 TO DATE)
18 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:231829

REFERENCE 2: 138:231828

REFERENCE 3: 137:288261

REFERENCE 4: 137:226940

REFERENCE 5: 136:242214

REFERENCE 6: 136:161536

REFERENCE 7: 135:127209

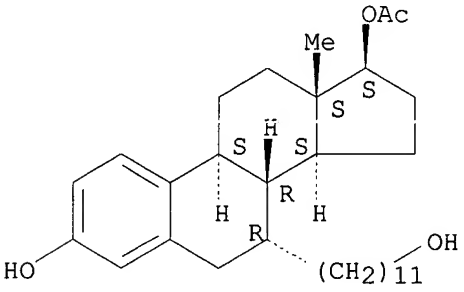
REFERENCE 8: 134:348617

REFERENCE 9: 134:275892

REFERENCE 10: 134:275891

L33 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **98008-57-2** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 7-(11-hydroxyundecyl)-, 17-acetate, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H48 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1962 TO DATE)
5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:77518

REFERENCE 2: 115:174681

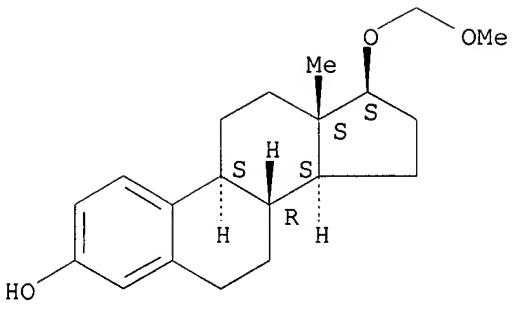
REFERENCE 3: 115:85452

REFERENCE 4: 112:70145

REFERENCE 5: 103:105214

L33 ANSWER 20 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **88899-72-3** REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(methoxymethoxy)-, (17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:107327

REFERENCE 2: 119:226237

REFERENCE 3: 108:150803

REFERENCE 4: 100:96847

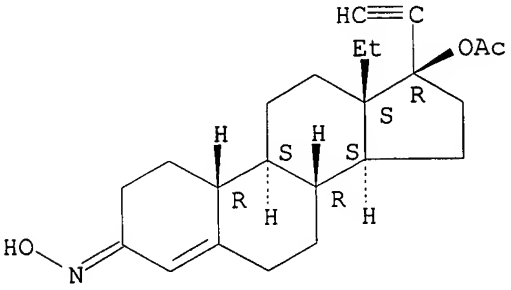
L33 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **79871-54-8** REGISTRY
CN 18,19-Dinorpregn-4-en-20-yn-3-one, 17-(acetyloxy)-13-ethyl-, 3-oxime, (17.alpha.)-, mixt. with (17.alpha.)-19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)-, mixt. contg. (9CI)
OTHER NAMES:
CN Cilest
CN Cileste
CN Dexnorgestrel acetime-ethinylestradiol mixt.
CN Ethinylestradiol-norgestimate mixt.
CN Norgestimate-ethinylestradiol mixt.
CN Ortho Cyclen
CN Ortho Cyclen 21
CN Ortho Cyclen 28
CN Ortho Tri-Cyclen
CN Ortho Tri-Cyclen 21
CN Ortho Tri-Cyclen 28
CN Pramino
CN Tri Cyclen
CN Tricilest
CN Tricileste
FS STEREOSEARCH
MF C23 H31 N O3 . C20 H24 O2
CI MXS
LC STN Files: ADISNEWS, BIOSIS, BIOTECHNO, CA, CAPLUS, CIN, DIOGENES, DRUGPAT, DRUGUPDATES, EMBASE, MEDLINE, MRCK*, PHARMASEARCH, PROMT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

CM 1

CRN 35189-28-7

CMF C23 H31 N O3

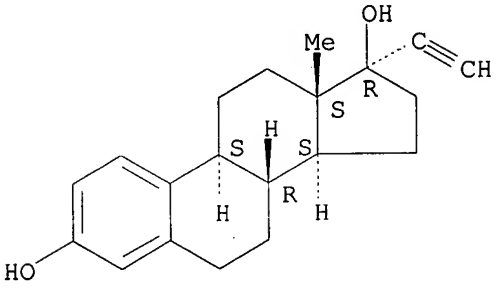
Absolute stereochemistry.
Double bond geometry unknown.



CM 2

CRN 57-63-6
CMF C20 H24 O2

Absolute stereochemistry.



37 REFERENCES IN FILE CA (1962 TO DATE)
37 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:163696

REFERENCE 2: 138:117749

REFERENCE 3: 138:33487

REFERENCE 4: 137:210420

REFERENCE 5: 137:156379

REFERENCE 6: 137:104002

REFERENCE 7: 137:104001

REFERENCE 8: 136:257419

REFERENCE 9: 136:160858

REFERENCE 10: 136:1101

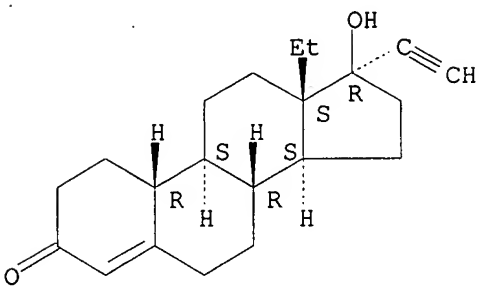
L33 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **8056-51-7** REGISTRY
CN 18,19-Dinorpregn-4-en-20-yn-3-one, 13-ethyl-17-hydroxy-,

(17.alpha.)-(.+-.)-, mixt. with (17.alpha.)-19-norpregna-1,3,5(10)-trien-20-yne-3,17-diol (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)-, mixt. contg. (9CI)
OTHER NAMES:
CN 17.alpha.-Ethynylestradiol-norgestrel mixt.
CN Biphasil
CN dl-Norgestrel-ethinylestradiol mixt.
CN dl-Norgestrel-ethynylestradiol mixt.
CN Duoluton
CN Ediwal
CN Ethinylestradiol-dl-norgestrel mixt.
CN Ethinylestradiol-norgestrel mixt.
CN Ethinylestradiol-norgestrel mixture
CN Ethynylestradiol-dl-norgestrel mixture
CN Ethynylestradiol-norgestrel mixt.
CN Ethynylestradiol-norgestrel mixture
CN Eugynon
CN Eugynon 30
CN Femenal
CN Follimin
CN Follinett
CN Follinyl
CN Gravistat
CN Lo-Femenal
CN Lo/Ovral
CN Microvlar
CN Microvlar 30
CN Neogynon
CN Neovletta
CN Nordiol
CN Norgestrel-ethynylestradiol mixt.
CN Orasecron
CN Ovidon
CN Ovral
CN Ovral 21
CN Ovral 28
CN Ovral L
CN Ovran
CN Primovlar
CN Pro-Duosterone
CN Rigevidon
CN Sequilar
CN Sequilarum
CN Sequostat
CN SH 71121
CN SHB 261AB
CN SHB 264AB
CN Stediril
CN Stediril d
CN Triovlar
CN WL 20
CN WL 33
CN WY-E 104
FS STEREOSEARCH
DR 8063-84-1, 8064-50-4, 70208-30-9
MF C21 H28 O2 . C20 H24 O2
CI MXS
LC STN Files: ADISNEWS, AGRICOLA, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CBNB, CHEMLIST, CIN, DIOGENES, EMBASE, MEDLINE, PHAR, PHARMASEARCH, PROMT, RTECS*, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

CM 1

CRN 6533-00-2
CMF C21 H28 O2

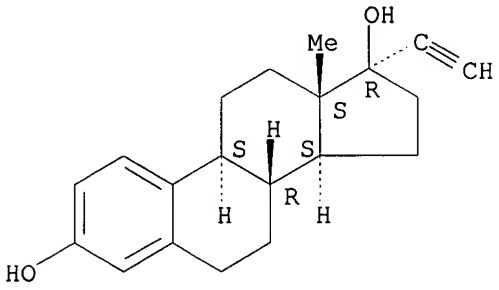
Relative stereochemistry.



CM 2

CRN 57-63-6
CMF C20 H24 O2

Absolute stereochemistry.



473 REFERENCES IN FILE CA (1962 TO DATE)
473 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:50049

REFERENCE 2: 137:833

REFERENCE 3: 136:364084

REFERENCE 4: 136:363962

REFERENCE 5: 136:319531

REFERENCE 6: 136:241828

REFERENCE 7: 136:212012

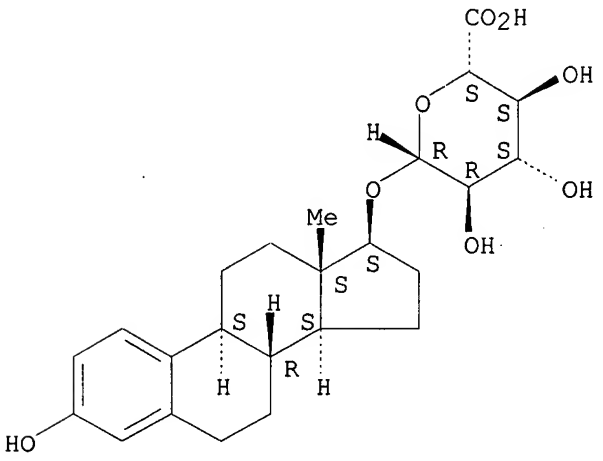
REFERENCE 8: 136:210698

REFERENCE 9: 136:112846

REFERENCE 10: 136:844

L33 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **1806-98-0** REGISTRY
CN .beta.-D-Glucopyranosiduronic acid, (17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estrane, .beta.-D-glucopyranosiduronic acid deriv.
CN Glucopyranosiduronic acid, 3-hydroxyestra-1,3,5(10)-trien-17.beta.-yl, .beta.-D- (6CI, 7CI, 8CI)
OTHER NAMES:
CN Estradiol 17-glucuronide
CN Estradiol 17.beta.-(.beta.-D-glucuronide)
CN Estradiol 17.beta.-glucuronide
FS STEREOSEARCH
DR 125926-20-7, 27851-73-6, 30137-07-6
MF C24 H32 O8
CI COM
LC STN Files: BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, DDFU, DRUGU, EMBASE, IPA, MEDLINE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

282 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
282 REFERENCES IN FILE CAPLUS (1962 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:233593

REFERENCE 2: 138:198339

REFERENCE 3: 138:185582

REFERENCE 4: 138:184677

REFERENCE 5: 138:102166

REFERENCE 6: 138:49551

REFERENCE 7: 138:16340

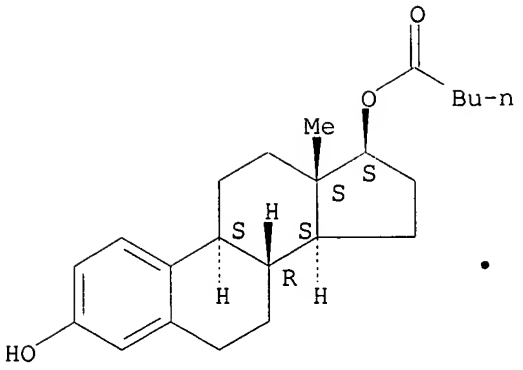
REFERENCE 8: 138:11194

REFERENCE 9: 138:2713

REFERENCE 10: 138:1537

L33 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **979-32-8** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17.beta.)-, 17-pentanoate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol valerate (6CI)
CN Estradiol, 17-valerate (7CI, 8CI)
OTHER NAMES:
CN 3-Hydroxy-17.beta.-valeroyloxyestra-1,3,5(10)-triene
CN Atladiol
CN Climaval
CN Deladiol
CN Delahormone unimatic
CN Delestrogen
CN Delestrogen 4x
CN Dura-Estradiol
CN Estra-1,3,5(10)-triene-3,17.beta.-diol 17-valerate
CN Estradiol 17.beta.-valerate
CN Estradiol valerianate
CN Estraval
CN Femogex
CN Gynogen LA
CN Gynogen LA 40
CN Neofollin
CN NSC 17590
CN Nuvelle
CN Oestradiol valerinate
CN Pelanin Depot
CN Pharlon
CN Primofol-Depot
CN Primogyn-Depot
CN Progynon-Depot
CN Progynova
CN Valergen
FS STEREOSEARCH
DR 907-12-0, 69557-95-5
MF C23 H32 O3
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CBNB, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, NIOSHTIC, PHARMASEARCH, PROMT, RTECS*, TOXCENTER, ULIDAT, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

777 REFERENCES IN FILE CA (1962 TO DATE)
8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
778 REFERENCES IN FILE CAPLUS (1962 TO DATE)
39 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:248709

REFERENCE 2: 138:231902

REFERENCE 3: 138:231901

REFERENCE 4: 138:158871

REFERENCE 5: 138:146907

REFERENCE 6: 138:101107

REFERENCE 7: 138:83614

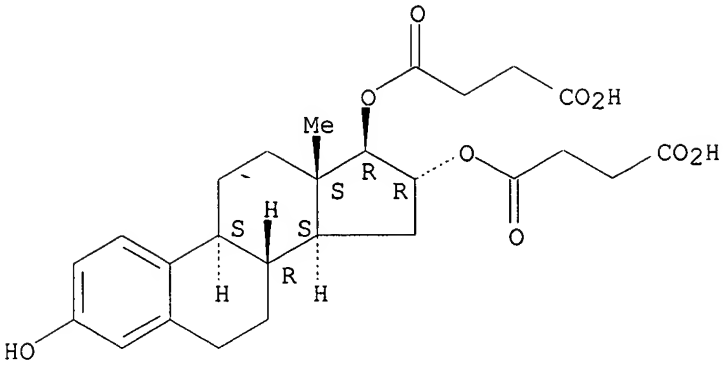
REFERENCE 8: 138:33532

REFERENCE 9: 137:363705

REFERENCE 10: 137:346927

L33 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **514-68-1** REGISTRY
CN Estra-1,3,5(10)-triene-3,16,17-triol, 16,17-bis(hydrogen butanedioate), (16.alpha.,17.beta.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estriol, 16,17-bis(hydrogen succinate) (7CI, 8CI)
CN Succinic acid, 16,17-diester with estriol (8CI)
OTHER NAMES:
CN Estriol 16,17-dihemisuccinate
CN Estriol succinate
CN Stiptanon
FS STEREOSEARCH
MF C26 H32 O9
CI COM
LC STN Files: ADISNEWS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CHEMLIST, DDFU, DRUGU, EMBASE, MEDLINE, TOXCENTER, USAN, USPATFULL
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

40 REFERENCES IN FILE CA (1962 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
40 REFERENCES IN FILE CAPLUS (1962 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:333525

REFERENCE 2: 137:237777

REFERENCE 3: 135:335171

REFERENCE 4: 135:111979

REFERENCE 5: 133:227817

REFERENCE 6: 131:189718

REFERENCE 7: 121:222993

REFERENCE 8: 121:222992

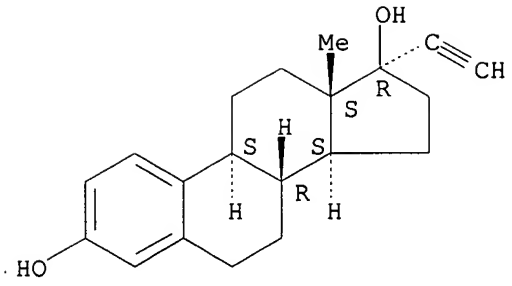
REFERENCE 9: 115:142307

REFERENCE 10: 115:45694

L33 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2003 ACS
RN **57-63-6** REGISTRY
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17.alpha.)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 19-Nor-17.alpha.-pregna-1,3,5(10)-trien-20-yne-3,17-diol (6CI, 7CI, 8CI)
OTHER NAMES:
CN 17-Ethinyl-3,17-estradiol
CN 17-Ethinylestradiol
CN 17-Ethynyl-3,17-dihydroxy-1,3,5-oestratriene
CN 17-Ethynylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17-Ethynylestradiol
CN 17-Nor-17.alpha.-pregna-1,3,5-(10)-trien-20-yne-3,17-diol
CN 17.alpha.-Ethinyl-1,3,5(10)-estratriene-3,17-diol
CN 17.alpha.-Ethinyl-17.beta.-estradiol
CN 17.alpha.-Ethinyl-3,17-dihydroxy-.DELTA.1,3,5-estratriene

CN 17.alpha.-Ethinylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17.alpha.-Ethinylestradiol
CN 17.alpha.-Ethynylestra-1,3,5(10)-triene-3,17.beta.-diol
CN 17.alpha.-Ethynylestradiol
CN 19-Nor-17.alpha.-pregna-1,3,5(10)-trien-20-yne-3,17.beta.-diol
CN Amenoron
CN Chee-O-Gen
CN Chee-O-Genf
CN Diogyn E
CN Dyloform
CN Esteed
CN Estigyn
CN Estinyl
CN Eston-E
CN Estoral
CN Estorals
CN Estradiol, 17-ethynyl-
CN Ethidol
CN Ethinoral
CN Ethinylestradiol
CN Ethinyloestradiol
CN Ethynylestradiol
CN Ethynyloestradiol
CN Eticyclin
CN Eticyclol
CN Etinestrol
CN Etinestryl
CN Etinoestryl
CN Etistradiol
CN Follicoral
CN Ginestrene
CN Inestra
CN Linoral
CN Lynoral
CN Menolyn
CN Microfollin
CN neo-Estrone
CN Novestrol
CN NSC 10973
CN Oradiol
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY
FS STEREOSEARCH
DR 77538-56-8, 406932-93-2
MF C20 H24 O2
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DIOGENES, DRUGNL, DRUGU, DRUGUPDATES, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PHAR, PROMT, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3971 REFERENCES IN FILE CA (1962 TO DATE)
80 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3974 REFERENCES IN FILE CAPLUS (1962 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:260224

REFERENCE 2: 138:259542

REFERENCE 3: 138:259505

REFERENCE 4: 138:255252

REFERENCE 5: 138:250058

REFERENCE 6: 138:248696

REFERENCE 7: 138:248678

REFERENCE 8: 138:248673

REFERENCE 9: 138:248406

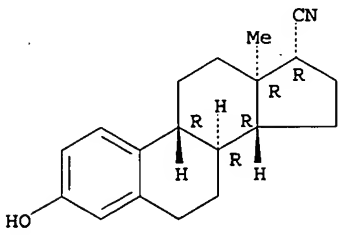
REFERENCE 10: 138:243401

10008569

=> d scan

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Estra-1,3,5(10)-triene-17-carbonitrile, 3-hydroxy-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.)- (9CI)
MF C19 H23 N O

Absolute stereochemistry. Rotation (-).

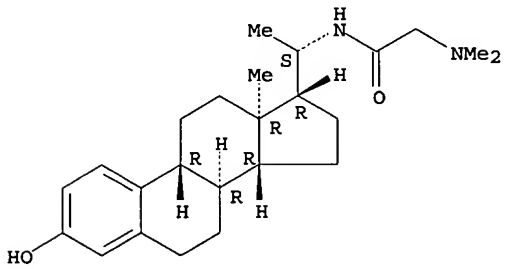


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):14

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Acetamide, 2-(dimethylamino)-N-[(8.alpha.,9.beta.,13.alpha.,14.beta.,17.al
pha.,20S)-3-hydroxy-19-norpregna-1,3,5(10)-trien-20-yl]- (9CI)
MF C24 H36 N2 O2

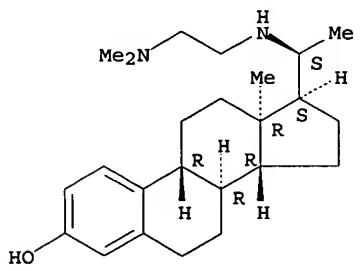
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[[2-(dimethylamino)ethyl]amino]-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,20S)- (9CI)
MF C24 H38 N2 O

Absolute stereochemistry.

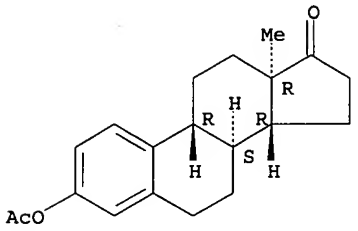


10008569

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Estra-1,3,5(10)-trien-17-one, 3-(acetyloxy)-,
(8.alpha.,9.beta.,13.alpha.,14.beta.)- (9CI)
MF C20 H24 O3

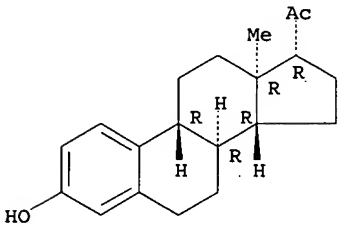
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-20-one, 3-hydroxy-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.)- (9CI)
MF C20 H26 O2

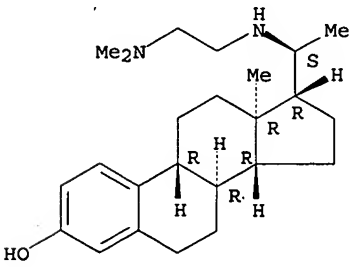
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[[2-(dimethylamino)ethyl]amino]-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.,20S)- (9CI)
MF C24 H38 N2 O

Absolute stereochemistry. Rotation (-).

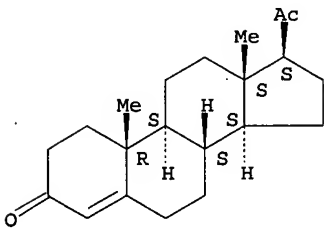


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10008569

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pregn-4-ene-3,20-dione (9CI)
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
MF C21 H30 O2
CI COM

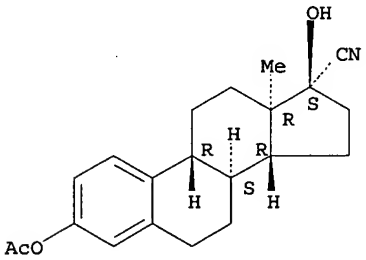
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Estra-1,3,5(10)-triene-17-carbonitrile, 3-(acetyloxy)-17-hydroxy-, (8.alpha.,9.beta.,13.alpha.,14.beta.,17.beta.)- (9CI)
MF C21 H25 N O3

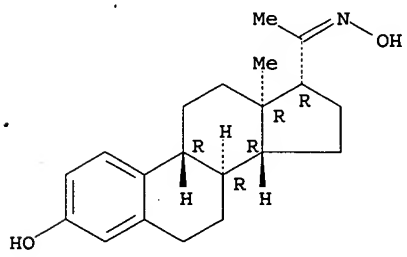
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-20-one, 3-hydroxy-, oxime, (8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.)- (9CI)
MF C20 H27 N O2

Absolute stereochemistry.
Double bond geometry unknown.

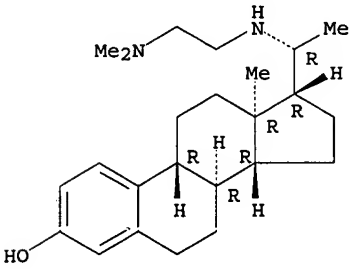


10008569

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[[2-(dimethylamino)ethyl]amino]-, (8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.,20R)- (9CI)
MF C24 H38 N2 O

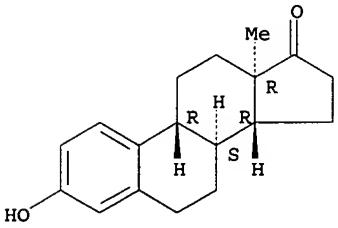
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-, (8.alpha.,9.beta.,13.alpha.,14.beta.)- (9CI)
MF C18 H22 O2

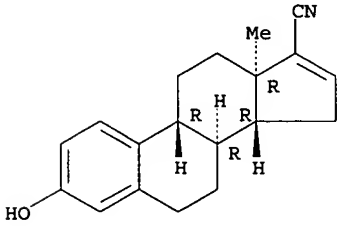
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Estra-1,3,5(10),16-tetraene-17-carbonitrile, 3-hydroxy-, (8.alpha.,9.beta.,13.alpha.,14.beta.)- (9CI)
MF C19 H21 N O

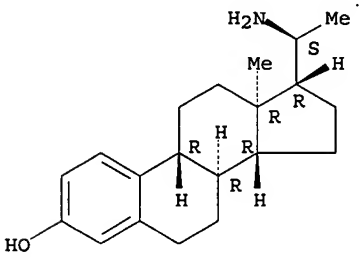
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-amino-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,17.alpha.,20S)- (9CI)
MF C20 H29 N O

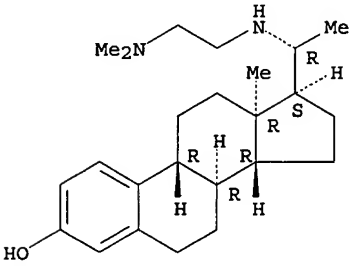
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

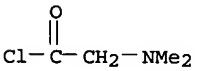
L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[[2-(dimethylamino)ethyl]amino]-,
(8.alpha.,9.beta.,13.alpha.,14.beta.,20R)- (9CI)
MF C24 H38 N2 O

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Acetyl chloride, (dimethylamino)-, hydrochloride (9CI)
MF C4 H8 Cl N O . Cl H



● HCl